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SUMMARY

A computer program written in FORTRAN IV language is presented which determines the performance of a shock tube for arbitrary equilibrium real gas mixtures. For specified initial gas composition and charging conditions, the program output includes velocity, pressure, density, enthalpy, temperature, sound speed, and species mole fractions at any point in the shock tube cycle.

Several representative calculations illustrate the utility of the program. The program is applicable to both simple and buffered shock tubes as well as to the expansion tube.

INTRODUCTION

The shock tube has been widely utilized as an experimental device for producing high enthalpy flows for research in such areas as aerodynamic testing, chemical kinetics, and radiation gas dynamics. Much of the utility of the shock tube is due to the capability of generating a broad range of test conditions in various gas mixtures.

Numerous current experimental investigations are being conducted in gas mixtures simulating planetary atmospheres that differ markedly from air. Before initiating a test program, it is essential to ascertain the theoretical performance of the shock tube for the particular gas mixture being used in order to aid in determining test conditions and in analyzing data. Previous shock tube performance investigations are too numerous to describe herein, but they generally can be divided into two classes. Both simple and buffered shock tubes are discussed in reference 1 and this study is an example of the analyses that assume a perfect gas throughout the operating cycle. In reference 2 an investigation of the expansion tunnel is presented and is illustrative of those analyses that treat the shocked gas in the driven chamber as a real gas in thermodynamic and chemical equilibrium, but the driver gas in the unsteady expansion process is assumed to be perfect. The rather exhaustive treatment of the perfect gas performance of the simple shock tube in reference 3 does, however, include a discussion of real gas effects.

It is desirable to construct a digital computer program to calculate shock tube performance for arbitrary driver and driven gases so that the gas at any point in the operating cycle may be treated either as a perfect gas or as an equilibrium real gas. This report describes such a program based upon the assumptions of inviscid one-dimensional flow, no mixing at the interfaces, and instantaneous diaphragm bursts. The program is applicable to simple or buffered shock tubes and expansion tubes. Performance parameters for some typical gas mixtures and operating conditions are presented to demonstrate the utility of the program.

SYMBOLS

a	sound speed, cm/sec
h	enthalpy, ergs/g
p	pressure, dynes/cm^2
p_o	standard atmospheric pressure, 1.01325×10^6 dynes/cm^2
R	universal gas constant, 8.31469×10^7 ergs/mole-^{o}K
s	entropy, ergs/g-^{o}K
T	temperature, ^{o}K
t	time, sec
u	flow speed, cm/sec
U_S	shock speed, cm/sec
x	distance, cm
γ	ratio of specific heats
μ	molecular weight

ρ	density, g/cm^3

Subscripts:

o	reference conditions
1	state of quiescent gas in front of normal shock
2	state of gas behind normal shock
3	state of expanded driver gas
4	initial driver gas conditions
5	state of test gas in expansion tube
10	state of quiescent gas in double-diaphragm shock tube

ANALYSIS

A distance-time diagram for the simple shock tube is schematically depicted in figure 1(a). Figure 1(b) illustrates the quiescent driver and test gases prior to diaphragm burst at $t = 0$. Figure 1(c) indicates the wave system at $t = t_a$. The test gas in state ① is compressed and heated by the normal shock wave to state ②, while the driver gas in state ④ undergoes an isentropic unsteady expansion to state ③.

In practice the shock tube is often designed to operate at a fixed driver pressure and the driven chamber pressure (and the buffer chamber pressure for the buffered shock tube) is adjusted to produce the desired test conditions. For specified initial charging conditions ① and ④, the unsteady expansion must be solved for state ③ and the normal shock wave must be solved for state ②. The respective solutions for states ② and ③ are compatible only when the pressures and velocities of the two states are equal (i.e., $p_2 = p_3$ and $u_2 = u_3$).

Unsteady Expansion

The governing differential equation (ref. 4) for an isentropic unsteady expansion is

$$du = \mp\left(\frac{dh}{a}\right)_s \tag{1}$$

where the negative and positive signs refer to upstream and downstream waves, respectively. Then, the velocity increment imparted to the flow by the expansion is

$$\Delta u = u_3 - u_4 = \mp \int_{h_4}^{h_3} \left(\frac{dh}{a}\right)_s \tag{2}$$

In order to relate the pressure and velocity in the as yet undetermined state ③ for an equilibrium real gas, it is necessary to resort to numerical techniques to evaluate the integral in equation (2). The analysis formulated herein utilizes the equilibrium program of reference 5. The program includes ionization and dissociation and involves the following assumptions:

(1) The mixture is composed of ideal gases.

(2) For diatomic species the rigid-rotor harmonic oscillator model is used with vibrational-rotational corrections for each electronic configuration.

(3) Only electronic levels with principal quantum number less than or equal to 5 are included.

The free energy of each of the species is determined from the partition function of quantum statistical mechanics. The equilibrium composition is then arrived at by minimization of free energy.

This program is used to generate an array of the thermodynamic state variables ρ, h, a, and s for the gas mixture over selected ranges of pressures and temperatures. Interpolation within the array permits tabulation of p, ρ, h, T, and a for constant $s = s_4$. The integral in equation (2) can then be evaluated by a second-order Gaussian quadrature (ref. 6) between limit h_4 and an assumed limit h_3. The pressure p_3 is then determined from the tabulation at the assumed h_3. It is thus possible to determine a unique correspondence between p_3 and u_3 at constant s_4.

For a perfect gas, equation (2) can be integrated in closed form to yield

$$p_3 = p_4 \left[1 - \frac{\gamma - 1}{2}\left(\frac{u_3 - u_4}{\sqrt{\frac{\gamma R T_4}{\mu}}}\right)\right]^{\frac{2\gamma}{\gamma - 1}} \tag{3}$$

Normal Shock Wave

The conservation equations valid across a moving normal shock wave are

$$\rho_1 U_S = \rho_2 \left(U_S - u_2\right) \tag{4}$$

$$p_1 + \rho_1 U_S^2 = p_2 + \rho_2 \left(U_S - u_2\right)^2 \tag{5}$$

$$h_1 + \frac{U_S^2}{2} = h_2 + \frac{\left(U_S - u_2\right)^2}{2} \tag{6}$$

The solution to equations (4) to (6) for an equilibrium real gas requires an iterative method to determine the pressure and velocity in state ②. This analysis utilizes the normal shock program of reference 7, which is based upon a free-energy minimization technique for calculating equilibrium thermodynamic state variables coupled with the conservation equations and a modified Newton-Raphson iteration method. The equilibrium thermochemical calculations involve the same assumptions as those in reference 5. For a specified state ① and incident shock velocity, this method determines p_2 and u_2. For a range of values of U_S, the correspondence between p_2 and u_2 can then be established.

For a perfect gas, the following relation between p_2 and u_2 can be readily derived:

$$u_2 = \frac{\sqrt{\frac{\gamma R T_1}{\mu}}}{\gamma}\left(\frac{p_2}{p_1} - 1\right)\left(\frac{\frac{2\gamma}{\gamma + 1}}{\frac{p_2}{p_1} + \frac{\gamma - 1}{\gamma + 1}}\right)^{1/2} \tag{7}$$

Method of Solution

The solution generated by the program described herein is based upon the previously noted requirement that p_3 equal p_2 and u_3 equal u_2. By following the method outlined for the solution of the unsteady expansion, a monotonically decreasing sequence of pressure as a function of velocity can be calculated. In similar fashion, the normal shock solution yields a monotonically increasing sequence of pressure as a function of velocity. The method of false position coupled with a Lagrangian interpolation (ref. 6) is then used to determine the crossover point of the two sequences. The crossover values of p and u are the required solution.

PROGRAM DESCRIPTION

For application to the simple shock tube (fig. 1), the program contains the four options corresponding to the combinations of either a real or perfect driver gas and either real or perfect driven gas. For the perfect gas option, it is only necessary to solve the closed-form equations (3) and (7) for the expansion and normal shock, respectively. For the perfect gas expansion, the required input consists of the initial conditions p_4, T_4, and u_4 and the constants μ_4, γ_4, and R; in addition, a range of velocities

$$u_4 < u_3 < u_4 + \frac{2}{\gamma - 1}\sqrt{\frac{\gamma R T_4}{\mu}}$$

is required to generate a velocity-pressure $\left(u_3\text{-}p_3\right)$ curve.

For the perfect gas normal shock, the required inputs are p_1, T_1, μ_1, R, γ_1, and a range of p_2 values

$$p_1 < p_2 < p_4$$

from which a pressure-velocity $\left(p_2\text{-}u_2\right)$ function is computed.

The real gas expansion calculation utilizes the program of reference 5 to generate thermodynamic data. In addition to the input required for the program of reference 5, suitable ranges of temperatures and pressures must be included to define the array of thermodynamic variables. For the constant entropy value s_4, the program reads from the array h as a function of 1/a and then performs the numerical integration

$$u_3 - u_4 = -\int_{h_4}^{h_3}\left(\frac{dh}{a}\right)_{s_4}$$

from which the pressure-velocity $\left(p_3\text{-}u_3\right)$ function is determined. The option exists for readout of velocity-pressure $\left(u_3\text{-}p_3\right)$ curves for various entropy values, as well as u_3 as a function of h and T, or for proceeding directly to the solution of the normal shock.

The program of reference 7 is used to determine equilibrium conditions behind a normal shock for a range of U_S values and for given p_1, T_1, and gas composition. Each U_S value thus leads to a value of p_2 and corresponding value of u_2, which define the pressure-velocity function to be matched to the velocity-pressure $\left(u_3\text{-}p_3\right)$ curve from the expansion calculation.

For expansion tube or buffered shock tube performance calculation, the program is applied twice to the simple shock tube cycle (fig. 2). The conditions behind the normal shock (state ②) in the first calculation become the driver gas conditions (state ④) for the second calculation. It should be noted that the driver velocity for the second calculation is no longer zero, since instantaneous diaphragm rupture has been assumed (i.e., no reflection). The fact that the gas behind the first incident shock in such a system may be dissociated and ionized emphasizes the necessity for a real gas calculation of the expansion phase.

The program FORTRAN listing and a flow chart are presented for reference in the appendix.

SAMPLE CALCULATIONS

Several sample calculations illustrate the application of the program to the determination of performance for single- and double-diaphragm shock tubes. The driver pressures chosen are such that intermolecular forces may be neglected and the assumption of a mixture of ideal gas is valid.

Figure 3 shows the velocity-pressure $(u_3\text{-}p_3)$ curve for the equilibrium real gas isentropic expansion of helium and the velocity-pressure $(u_2\text{-}p_2)$ curves for normal shock waves in equilibrium air for four initial driven chamber pressures with $T_1 = 300^\circ$ K. The helium driver conditions chosen are $T_4 = 15\ 000^\circ$ K and $p_4/p_o = 315$. The cross-over point of the curves determines $p_3 = p_2$ and $u_3 = u_2$ for each driver-driven configuration. From these results the shock speeds corresponding to each calculation may be evaluated. The performance plot of $U_{S,1}$ as a function of p_1/p_o for these driver conditions is given in figure 4.

Figures 5 to 9 illustrate a typical set of performance calculations for the expansion tube. This type of facility (ref. 8) consists of three sections separated by two destructible diaphragms as shown in figure 2. One section contains the driver gas (④), the intermediate section contains the test gas (①), and the remaining section contains the accelerating gas (⑩).

For the performance calculations, the simple shock tube cycle was applied first to regions ④ and ① in order to obtain conditions in region ② . Then the calculation was repeated, with conditions in region ② as the driver and the gas in region ⑩ as the driven gas, which led to the determination of the test gas conditions in region ⑤.

The following initial conditions were chosen for these computations:

$$\frac{p_4}{p_o} = 30; \quad T_4 = 2500^\circ \text{ K; helium (perfect gas)}$$

$$10^{-3} \leqq \frac{p_1}{p_o} \leqq 10^{-1}; \quad T_1 = 300^\circ \text{ K; air (real gas)}$$

$$10^{-3} \leqq \frac{p_{10}}{p_o} \leqq 10^{-2}; \quad T_{10} = 300^\circ \text{ K; helium (perfect gas)}$$

In this calculation the temperatures experienced by the helium were not great enough to cause a noticeable departure from perfect gas behavior. Figure 5 shows the shock speed in air $U_{S,1}$ as a function of p_1/p_0 resulting from the first diaphragm burst. The final shock speed in helium in the accelerating chamber is shown in figure 6 for $\frac{p_{10}}{p_0} = 5 \times 10^{-4}$, 10^{-3}, and 5×10^{-3}. The conditions of most interest for this facility are those of the gas in region ⑤, which has been shocked in the first cycle and expanded and cooled in the second cycle. The test gas conditions which may be obtained from the given initial conditions are shown in figures 7, 8, and 9. As would be expected, the families of curves for shock speed $U_{S,10}$ and test gas speed u_5 are similar (figs. 6 and 7). The performance data indicate that the facility may be operated in a manner in which the test gas speed and pressure do not change appreciably although the temperature may vary from several thousand degrees to several hundred degrees Kelvin.

This program was also used to make a set of calculations for the 3.8-inch double-diaphragm shock tube at the Langley Research Center in order to predict the real gas performance for a test gas mixture of 90 percent N_2 and 10 percent CO_2. The calculations for a double-diaphragm, or buffered, shock tube are carried out in the same manner as those described for the expansion tube. However, in this facility the test gas is contained in the third chamber instead of in the intermediate section; hence, the results of primary interest are the shock speeds in the test gas for a range of p_1/p_o and p_{10}/p_o, which are shown in figures 10 and 11.

Figure 10 gives the performance of this shock tube for the following initial conditions:

$\frac{p_4}{p_o} = 100$; $T_4 = 300^o$ K; helium (perfect gas)

$5 \times 10^{-2} \leqq \frac{p_1}{p_o} \leqq 5$; $T_1 = 300^o$ K; helium (perfect gas)

$5 \times 10^{-4} \leqq \frac{p_{10}}{p_o} \leqq 5 \times 10^{-2}$; $T_{10} = 300^o$ K; 90 percent N_2 and 10 percent CO_2 (real gas)

Figure 11 shows the performance for these same initial conditions for gases in regions ① and ⑩ but with perfect hydrogen used instead of helium for gas in region ④. It has been observed experimentally that for the initial conditions for which this facility is operated, the performance calculations give a reasonably accurate prediction of actual behavior.

The results of all sample calculations were checked where possible with the results of references 1, 2, 4, 7, and 8. In all calculations agreement was within 1 percent.

RÉSUMÉ

A computer program written in FORTRAN IV language is presented which determines the performance of a shock tube for arbitrary equilibrium real gas mixtures. For specified initial gas composition and charging conditions, the program output includes velocity, pressure, density, enthalpy, temperature, sound speed, and species mole fractions at any point in the shock tube cycle.

Several representative calculations illustrate the utility of the program. It was noted that these calculations agreed with results of other investigations.

It may be concluded that the program has both generality and flexibility for computing shock tube performance in arbitrary gas mixtures.

Langley Research Center,
National Aeronautics and Space Administration,
Langley Station, Hampton, Va., June 10, 1968,
129-01-03-10-23.

APPENDIX

SHOCK TUBE PERFORMANCE PROGRAM LISTING AND FLOW CHART

The FORTRAN listing and a schematic flow diagram of the program are presented. The program is composed of nine subroutines as follows:

(1) PEREX – Computes p_3 as a function of u_3 for a given p_4, u_4, T_4, and R

(2) ROGO – Computes an array of thermodynamic state variables for a given range of p and T (program of ref. 5)

(3) INTER – Uses a three-point Aitkens interpolation formula to find p, h/RT, and a/a_o at constant $(s/R)_4$

(4) INTEG – Computes $\int \frac{dh}{a}$ by Gaussian quadrature

(5) PERNS – Computes u_2 for a given p_1, p_2, T_1, γ_1, μ_1, and R

(6) NORMAL – With given p, T_1, and u, computes normal shock properties of gas

This subroutine makes use of an equilibrium program which computes thermodynamic properties of a gas at a given T and p (program of ref. 7).

(7) SOLUT – Given (p_2,u_2) and (p_3,u_3), finds solution to curves

(8) FTLUP – Uses Aitkens interpolation formula for three points; finds U_S to correspond to u_2

(9) SLITE – Sets a flag to be checked later on in subroutine

Subroutines (1) to (4) apply to the expansion phase only and the program may be stopped at this point. Also, u_3, p_3, T_3, $(h/RT)_3$, and $(a/a_o)_3$ may be punched out to save for later computer runs so that the curves do not have to be recomputed. Subroutines (5) to (9) apply to the normal shock portion of the program.

The program listing and flow chart are reproduced in the following pages.

APPENDIX

```
      PROGRAM D1282(INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9)
      REAL MU
      INTEGER PUN,COMPUT,REAL,EXPO
      DIMENSION AM(30),HM(30)
C
C     INPUT FOR EXPANSION - REAL GAS
C
      COMMON PN(30),TM(30),NUMT,NCAPX,SOR4,U4
C
C     INPUT FOR EXPANSION - PERFECT GAS
C
      COMMON  P4,T4,U3(30)
C
C     INPUT  CODES
C
      COMMON  PUN,EXPO,REAL , COMPUT
C
C     INPUT FOR NORMAL SHOCK
C
      COMMON P1,T1,P2(30),NUMP,USTO(30),U2(30)
      COMMON ISPEC(30),JMOL(10),M,N,BETA(5),NS,
     1AMC,NB,NBTA(5)
C
C     INPUT FOR PERFECT   EXPANSION AND SHOCK
C
      COMMON MU,GAMMA,R
C
C     GAS NAME
C
      COMMON NAME(10)
C
      COMMON/BLOCK/HM,AM,MM,P3(30)
C
      NAMELIST/EXP/PN,TM,NUMT,NCAPX,SOR4,U4,P4,T4,U3,MU,GAMMA,R,PUN,
     1EXPO,REAL,COMPUT
      NAMELIST/NORMS/P1,T1,P2,NUMP,USTO,U2,ISPEC,JMOL,M,N,BETA,NS,NB,
     1NBTA,MU,GAMMA,R,REAL,COMPUT
      EXPO=1
      CALL SLITE(1)
      NS=0
      REAL =0
      COMPUT=0
    1 READ(5,2010)NAME
 2010 FORMAT(10A6)
      READ(5,EXP)
      WRITE(6,2008)
 2008 FORMAT(31H1SHOCK TUBE PERFORMANCE PROGRAM//14H ENG. J. NEALY,10X,
     115HPROG. J. KEMPER)
C
C      IF( COMPUT =1, OR 0  READ IN U3,P3 , COMPUTE U3, P3
C
       IF(COMPUT.EQ.0) GO TO 10
C
C     READ IN U3,P3
C
       IF(REAL.EQ.1) GO TO 5
       READ(5,2005) SOR4,U4
 2005  FORMAT(14X,E15.8,5X,E15.8)
       GO TO 6
    5  READ(5,2006) P4,T4
 2006  FORMAT(16X,E15.8,5X,E15.8)
    6  READ(5,2007) (P3(I),I=1,NUMT)
 2007  FORMAT(4E17.8)
       READ(5,2007)  (U3(I),I=1,NUMT)
       GO TO 101
   10  CONTINUE
C
C      IF REAL =0,1   REAL, OR PERFECT GAS
C
       IF(REAL.EQ.0) GO TO 15
       CALL PEREX(P4,U4,GAMMA,R,T4,MU,U3,NUMT,P3)
       GO TO 101
   15  CALL ROGO(PN,TM,NUMT,NCAPX,GAMMA,SOR4 )
       MM=NUMT
       CALL INTEG(U3,U4)
       WRITE(6,201) SOR4,(I,TM(I),P3(I),HM(I),AM(I),U3(I),I=1,NUMT)
  201  FORMAT(7H1OUTPUT/15X,4HS/R=E14.7/3H M ,2X,8X,1HT,8X,10X,1HP,
      118X,1HH,18X,1HA,
      118X,2HU3/(I3,5(2X,E17.8)))
  101  IF(PUN.EQ. 1) GO TO 110
  100  WRITE(6,2009)P4,T4,(U3(I),P3(I),I=1,NUMT)
 2009  FORMAT(1H1,2X,3HP4=E15.7,2X,3HT4=E15.7/8X,2HU3,17X,2HP3/
      1(E17.8,2X,E17.8))
  102  IF(EXPO.EQ.1) GO TO 150
       GO TO 1
C
C      PUNCH U3,P3
C
  110  IF(REAL.EQ.0) GO TO 111
       PUNCH 2000,P4,T4
 2000 FORMAT(11HPERFECT GAS,2X,3HP4=E15.8,2X,3HT4=E15.8)
      GO TO 112
  111 PUNCH 2001, SOR4,U4
 2001 FORMAT(8HREALGAS,2X,4HS/R=E15.8,2X,3HU4=E15.8)
  112 PUNCH 2003,(P3(I),I=1,NUMT)
 2003 FORMAT(4E17.8,4X,2HP3)
      PUNCH 2004,(U3(I),I=1,NUMT)
 2004 FORMAT(4E17.8,4X,2HU3)
C

      GO TO 102
C
C     NORMAL SHOCK
C
  150 READ(5,NORMS)
      CALL SLITE(2)
 1515 WRITE(6,206)NAME,P4,T4,T1
  206 FORMAT(7H1OUTPUT/1H0,9X,2HP4,17X,2HT4,17X,2HT1,20X,10A6/
     X3(E17.8,2X)//7X,2HP1
     1,17X,2HUS,17X,2HU2,17X,2HP2//)
      IC=1
  159 IF(COMPUT.EQ.0) GO TO 160
      GO TO 165
  160 IF(REAL.EQ.0)GO TO 164
  161 CALL PERNS(P1,T1,GAMMA,MU,R,P2,U2,NUMP)
      GO TO 165
  164 CALL NORMAL(P1,T1)
  165 CALL SOLUT(U3,P3,U2,P2,NUMT,NUMP,U,P)
      IF(REAL.EQ.0) GO TO 170
      UP=SQRT(GAMMA*R*T1/MU)*(SQRT(1.+(P/P1-1.)*(GAMMA+1.)/(2.*GAMMA)))
      UP=UP/30.48
      GO TO 175
  170 CALL FTLUP(U,UP,-1,NUMP,U2,USTO)
  175 CONTINUE
      IF(NS.EQ.1) WRITE(6,4456)
      WRITE(6,207)P1,UP,U,P
  207 FORMAT(4(E17.8,2X))
      IF(NS.EQ.1) WRITE(6,4456)
 4456 FORMAT(//)
      PLAST=P1
C
C     READ NEXT P
      READ(5,NORMS)
      IF(P1.EQ.PLAST) GO TO 1
      GO TO 159

      END
```

```
$IBFTC PEREX   DECK
      SUBROUTINE PEREX(P4,U4,GAMMA,R,T4,MU,U3,M,P3)
      DIMENSION U3(30),P3(30)
      REAL MU
      GAMY=2.*GAMMA/(GAMMA-1.)
      P4=P4*1.01325E6
      DO 10 I=1,M
      P3(I)=P4*(1.-(GAMMA-1.)/2.*(((U3(I)-U4)*30.48)/SQRT(GAMMA*R*T4/MU)
     1))**GAMY
   10 P3(I)=P3(I)/1.01325E6
      P4=P4/1.01325E6
      RETURN
      END
```

```
$IBFTC ROGO    LIST
      SUBROUTINE ROGO(PN,TM,NUMT,NCAPX,GAM,SOR4)
C     PERRY NEWMAN,EQUILIBRIUM THERMODYNAMIC PROPERTIES WITH DERIVATIVES
   80 FORMAT(2I5,2E14.8)
   81 FORMAT(A6,3I5,3E14.8)
   82 FORMAT(5E14.8)
   83 FORMAT(E14.8,2I5)
   84 FORMAT(4E14.8,I5)
   90 FORMAT(//4H MU=E15.8,2X,3HPO=E15.8,2X,5HRHOO=E15.8,2X,3HAO=E15.8)
   93 FORMAT(/(8E16.8))
   97 FORMAT(//,1X6HA(I,J),2X2HI=I4,2X2HJ=I4/(8E16.8))
   98 FORMAT(1X2HP=E15.8,2X28H100 ITERATIONS-NONCONVERGENT)
  100 FORMAT(16H1EXPANSION PHASE)
  101 FORMAT(75H0EQUILIBRIUM THERMODYNAMIC PROPERTIES WITH DERIVATIVES
     1 IN REAL GAS SYSTEM//)
  999 FORMAT(/)
 1000 FORMAT(1H1,57X2HT=I5,1X1HK,//)
 1001 FORMAT(6X3HLOG,5X3HLOG,7X1HZ,9X4HH/RT,6X3HS/R,6X3HLOG,6X6HDRHODT,5
     1X6HDRHODP,3X4HCP/R,6X4HCV/R,5X5HGAMMA,3X6HGAMMAE,3X4HA/AO/5X4HP/PO
     2,3X8HRHO/RHOO,34X2HNE,5X7H(T/RHO),4X7H(P/RHO)//)
 1002 FORMAT(F9.1,F10.4,F9.4,F11.4,F10.4,F9.3,F10.3,F10.3,F10.3,F10.3,F8
     1.3,F8.3,F9.3)
      REAL    NO,M,LAMB,LAMBDA,MU,NE,NEGFRT,LOGNE,MASSFR,LMIN
      INTEGER F(30),V(30,10),PUN
      DIMENSION SPECIE(30),LB(30),M(30),DELHF(30),BETA(30),NDEBUG(30)
     1,IPIVOT(10),R(10,10),SUMAY(10,1),G(30,30),E(30,30),BE(30,10),ALPHA
     2E(30,10),OMEGA(30,10),OMEGAX(30,10),          XOMEG(30,4),XOMEGX(30
     3,4),Z(30),SIGMA(10),U(10),DELTA(10),GAMMA(10),XX(10),Q(30),Y(30),X
     4(30),A(30,9),HORT(30),FORT(30),NEGFRT(30),PI(9,2),XPRIME(30),MASSF
     5R(30),CAPX(50),YINT(30,1),CSUBP(30),PSI(30,2),CON(10,2),DXDT(30),R
     6R(10,10),O(10,10),ABL(30),SBL(30),HBL(30),PN(30),TM(30)
      WRITE(6,100)
      WRITE(6,101)
      CALL SLITET(1,JJ)
      IF(JJ.EQ.2) GO TO 7777
      H=6.62517E-27
      XK=1.38044E-16
      PREF=1.013250E+6
      NO=6.02322E+23
      C=2.99793E+10
    1 READ(5,80) NUMSP,JINDX,EA,ER
C     IF NDEBUG EQUALS 0, DEBUG
      DO 3 I=1,NUMSP
      READ(5,81)SPECIE(I),LB(I),F(I),NDEBUG(I),M(I),DELHF(I),BETA(I)
      IL=LB(I)
      READ(5,82) (G(I,L),E(I,L),L=1,IL)
      IF(F(I).EQ.0) GO TO 3
      IF(F(I).EQ.2) GO TO 123
      READ(5,84)(BE(I,L),ALPHAE(I,L),OMEGA(I,L),OMEGAX(I,L),V(I,L),L=1,I
     1L)
      GO TO 3
  123 READ(5,82) BE(I,1),ALPHAE(I,1)
      READ(5,82)(XOMEG(I,LW),XOMEGX(I,LW),LW=1,4)
    3 CONTINUE
      READ(5,82) MU,(YINT(I,1),I=1,NUMSP)
      READ(5,82)((A(I,J),J=1,JINDX),I=1,NUMSP)
 7777 CONTINUE
      RHOO=PREF*MU/(NO*XK*273.15)
      AO=SQRT(GAM  *(PREF/RHOO))
      WRITE(6,90) MU,PREF,RHOO,AO
      DO 278 KP=1,NCAPX
  278 CAPX(KP)=ALOG10(PN(KP))
  279 DO 19 KI=1,NUMT
      T=TM(KI)
      KT=T
      WRITE(6,1000) KT
      WRITE(6,1001)
      NY=1
      PART=H*C/(XK*T)
      DO 9 I=1,NUMSP
      IL=LB(I)
      IF(F(I).EQ.1) GO TO 111
      IF(F(I).EQ.2) GO TO 112
      QSUM=0.
      FPQSUM=0.
      SPQSUM=0.
      DO 2 L=1,IL
      Z(L)=PART*E(I,L)
      GEZ=G(I,L)*EXP(-Z(L))
      QSUM=QSUM+GEZ
      FPQSUM=FPQSUM+GEZ*Z(L)
    2 SPQSUM=SPQSUM+(Z(L)-2.)*GEZ*Z(L)
      FPQSUM=FPQSUM/T
      SPQSUM=SPQSUM/T**2
      QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T
      GO TO 71
  111 QSUM=0.
      FPQSUM=0.
      SPQSUM=0.
      DO 11 L=1,IL
      Z(L)=PART*E(I,L)
      SIGMA(L)=PART*(BE(I,L)-.5*ALPHAE(I,L))
      U(L)=PART*(OMEGA(I,L)-2.*OMEGAX(I,L))
      DELTA(L)=ALPHAE(I,L)*1./(BE(I,L)-.5*ALPHAE(I,L))
      GAMMA(L)=(BE(I,L)/OMEGA(I,L))**2*1./(1.-.5*ALPHAE(I,L)/BE(I,L)'
      XX(L)=OMEGAX(I,L)/(OMEGA(I,L)-2.*OMEGAX(I,L))
      THREE=0.
      FOUR=0.
      FIVE=0.
      NV=V(I,L)+1
      DO 4 IV=1,NV
      W=IV-1
      CC=(1.-W*DELTA(L))
      AA=SIGMA(L)*CC
      BB=U(L)*(W-XX(L)*W*(W-1.))
      ONE1=1./AA+8.*GAMMA(L)/(AA**2*CC)+.33333333+AA/12.
      TWO2=1./AA+16.*GAMMA(L)/(AA**2*CC)-AA/12.-384.*GAMMA(L)**2/(AA**3*
     1CC**2)
      THREE=THREE+ONE1*EXP(-BB)
      FOUR=FOUR+(BB*ONE1+TWO2)*EXP(-BB)
    4 FIVE=FIVE+((BB**2*ONE1+2.*BB*TWO2+GAMMA(L)/(AA**2*CC)*(48.-3456.*G
     1AMMA(L)/(AA*CC)+46080.*GAMMA(L)**2/(AA**2*CC**2))+2./AA)*EXP(-BB))
      GEZ=G(I,L)*EXP(-Z(L))
      Q(L)=THREE/BETA(I)*GEZ
      QSUM=QSUM+Q(L)
      FPQSUM=FPQSUM+(FOUR+THREE*Z(L))*GEZ
   11 SPQSUM=SPQSUM+(Z(L)*(Z(L)-2.)*THREE+2.*(Z(L)-1.)*FOUR+FIVE)*GEZ
      FPQSUM=FPQSUM/(T*BETA(I))
      SPQSUM=SPQSUM/(T**2*BETA(I))
      QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T
      GO TO 71
  112 SIGMA(1)=PART*(BE(I,1)-.5* ALPHAE(I,1))
      PROD=1.
      SUM1=0.
      SUM2=0.
      DO 32 LW=1,4
      U(LW)=PART*(XOMEG(I,LW)-XOMEGX(I,LW))
      PROD=PROD*(1.-EXP(-U(LW)))
      BTM=EXP(U(LW))-1.
      SUM1=SUM1+U(LW)/BTM
   32 SUM2=SUM2+U(LW)**2*EXP(U(LW))/BTM**2
      QSUM=G(I,1)/(BETA(I)*SIGMA(1)*PROD)
      FPQSUM=(1.+SUM1)*QSUM/T
      SPQSUM=(SUM1**2+SUM2)*QSUM/T**2
      QI=(M(I)*T*.32807618)**1.5*QSUM*.13623883*T
   71 HORT(I)=2.5+T/QSUM*FPQSUM+DELHF(I)/(NO*XK*T)
      FORT(I)=DELHF(I)/(NO*XK*T)-ALOG(QI)
      NEGFRT(I)=-FORT(I)
    9 CSUBP(I)=2.5+2.*T/QSUM*FPQSUM-(T*FPQSUM/QSUM)**2+T**2*SPQSUM/QSUM
      NNN=1
      DO 39 KP=1,NCAPX
 9500 P=(10.**CAPX(KP))*PREF
      NYY=NY
      DO 500 I=1,NUMSP
  500 Y(I)=YINT(I,NY)
 9501*NUMIT=0***^^*
      MM=JINDX+1
      DO 301 J=1,JINDX
      O(J,MM)=0.
      DO 60 I=1,NUMSP
   60 O(J,MM)=O(J,MM)+A(I,J)*Y(I)
      O(MM,J)=O(J,MM)
  301 CONTINUE
      O(MM,MM)=0.
   50 CONTINUE
      YBAR=Y(1)
      NUMIT=NUMIT+1
      IF(NUMIT.EQ.101) GO TO 390
      DO 5 I=2,NUMSP
    5 YBAR=YBAR+Y(I)
      DO 7 K=1,JINDX
      R(1,K)=0.
      DO 6 I=1,NUMSP
    6 R(1,K)=R(1,K)+A(I,1)*A(I,K)*Y(I)
    7 CONTINUE
      ICOUNT=1
      JJ=2
      DO 28 J=JJ,JINDX
      DO 18 K=J,JINDX
      R(J,K)=0.
      DO 8 I=1,NUMSP
    8 R(J,K)=R(J,K)+A(I,J)*A(I,K)*Y(I)
   18 CONTINUE
      DO 10 K=1,ICOUNT
   10 R(J,K)=R(K,J)
      ICOUNT=ICOUNT+1
   28 JJ=1+ICOUNT
      DO 3011 J=1,MM
      R(J,MM)=O(J,MM)
 3011 R(MM,J)=O(J,MM)
```

```
      DO 302 J=1,MM
      DO 302 K=1,MM
  302 RR(J,K)=R(J,K)
      PYBAR=PREF*YBAR
      DO 304 J=1,JINDX
      SUMAY(J,1)=0.
      DO 303 I=1,NUMSP
      THIS=P*Y(I)/PYBAR
      IF(THIS.LE.0.) GO TO 303
      SUMAY(J,1)=SUMAY(J,1)+A(I,J)*Y(I)*(FORT(I)+ALOG(THIS))
  303 CONTINUE
  304 CONTINUE
      SUMAY(MM,1)=0.
      DO 305 I=1,NUMSP
      THIS=P*Y(I)/PYBAR
      IF(THIS.LE.0.) GO TO 305
      SUMAY(MM,1)=SUMAY(MM,1)+Y(I)*(FORT(I)+ALOG(THIS))
  305 CONTINUE
      MN=1
      NMAX=10
      CALL SIMEQ(R,MM,SUMAY,MN,DETERM,IPIVOT,NMAX,ISCALE)
      DO 306 J=1,JINDX
  306 PI(J,1)=SUMAY(J,1)
      U=SUMAY(MM,1)
      LMIN=1.
      LCOUNT=0
      DO 40 I=1,NUMSP
      API=0.
      DO 401 J=1,JINDX
  401 API=API+A(I,J)*PI(J,1)
      THIS=P*Y(I)/PYBAR
      IF(THIS.LE.1.E-38) GO TO 402
      X(I)=Y(I)*(NEGFRT(I)-ALOG(THIS)+U+1.+API)
      GO TO 403
  402 X(I)=0.
  403 IF(X(I)) 20,30,40
   20 LAMB=-Y(I)/(X(I)-Y(I))
      IF(LAMB.GT.0.)GO TO 21
      Y(I)=0.
      GO TO 50
   21 LCOUNT=1
      LMIN=AMIN1(LMIN,LAMB)
      GO TO 40
   30 IF(Y(I).EQ.0.)GO TO 40
      LCOUNT=1
      LAMB=1.
      LMIN=AMIN1(LMIN,LAMB)
      GO TO 40
   40 CONTINUE
      IF(LCOUNT.EQ.0)GO TO 51
      LAMBDA=.999999*LMIN
      DO 41 I=1,NUMSP
   41 Y(I)=(1.-LAMBDA)*Y(I)+LAMBDA*X(I)
      GO TO 50
   51 DO 52 I=1,NUMSP
      IF(Y(I).EQ.0.)GO TO 52
      IF(ABS(X(I)-Y(I))/Y(I).GE.ER.OR.ABS(X(I)-Y(I)).GE.EA)GO TO 53
   52 CONTINUE
      GO TO 29
   53 XBAR=0.
      LAMBDA=1.
      LASTCT=0
  531 DO 54 I=1,NUMSP
      XPRIME(I)=(1.-LAMBDA)*Y(I)+LAMBDA*X(I)
   54 XBAR=XBAR+XPRIME(I)
      DFLAMB=0.
      DO 541 I=1,NUMSP
      THIS=P*XPRIME(I)/(PREF*XBAR)
      IF(THIS.LE.0.) GO TO 541
      DFLAMB=DFLAMB+(X(I)-Y(I))*(FORT(I)+ALOG(THIS))
  541 CONTINUE
      IF(DFLAMB.GT.0.)GO TO 56
  542 DO 55 I=1,NUMSP
   55 Y(I)=XPRIME(I)
      GO TO 50
   56 LASTCT=LASTCT+1
      IF(LASTCT.EQ.4)GO TO 542
      LAMBDA=.9*LAMBDA
      XBAR=0.
      GO TO 531
   29 XBAR=0.
      ONE=0.
      TWO=0.
      DO 57 I=1,NUMSP
      XBAR=XBAR+X(I)
      ONE=ONE+X(I)*HORT(I)
      MASSFR(I)=X(I)*M(I)
      IF(Y(I).EQ.0.) GO TO 57
      TWO=TWO+X(I)*(FORT(I)+ALOG(X(I)))
   57 CONTINUE
```

```
      RECIPZ=1./(MU*XBAR)
      CAPU=CAPX(KP)+ALOG10(RECIPZ*273.15/T)
      CHORT=MU*ONE
      SOR=CHORT        -MU*(XBAR*ALOG(P/(PREF*XBAR))+TWO)
      RHO=P/(XBAR*NO*XK*T)
      NE=X(1)*RHO*NO
      IF(X(1).GT.(6.*10.**(-11))) GO TO 58
      LOGNE=-0.
      GO TO 391
   58 LOGNE=ALOG10(NE)
   59 GO TO 391
  390 WRITE(6,98)P
      GO TO 39
  391 CONTINUE
      DO 600 I=1,NUMSP
      TEST=X(I)*P/(XBAR*PREF)
      IF(TEST.LT.10.**(-20)) GO TO 601
      PSI(I,1)=X(I)/T*(HORT(I)-FORT(I)-ALOG(TEST))
      PSI(I,2)=-X(I)
      GO TO 600
  601 PSI(I,1)=0.
      PSI(I,2)=0.
  600 CONTINUE
      DO 602 J=1,JINDX
      CON(J,1)=A(1,J)*PSI(1,1)
      CON(J,2)=A(1,J)*PSI(1,2)
      DO 603 I=2,NUMSP
      CON(J,1)=CON(J,1)+A(I,J)*PSI(I,1)
  603 CON(J,2)=CON(J,2)+A(I,J)*PSI(I,2)
  602 CONTINUE
      CON(MM,1)=PSI(1,1)
      CON(MM,2)=PSI(1,2)
      DO 607 I=2,NUMSP
      CON(MM,1)=CON(MM,1)+PSI(I,1)
  607 CON(MM,2)=CON(MM,2)+PSI(I,2)
      NC=2
      CALL SIMEQ(RR,MM,CON,NC,DETERM,IPIVOT,NMAX,ISCALE)
      DO 604 J=1,MM
      PI(J,1)=CON(J,1)
  604 PI(J,2)=CON(J,2)
      DHDT=0.
      DO 605 I=1,NUMSP
      SUMAP=A(I,1)*PI(1,1)
      DO 606 J=2,JINDX
  606 SUMAP=SUMAP+A(I,J)*PI(J,1)
```

```
      DXDT(I)=PSI(I,1)-X(I)*(PI(MM,1)+SUMAP)
  605 DHDT=DHDT+(X(I)*CSUBP(I)+       T*HORT(I)*DXDT(I))
      DRHODT=T*PI(MM,1)-1.
      DRHODP=1.+  PI(MM,2)
      CPOR=MU*DHDT
      XZ=XBAR*MU
      CVOR=CPOR-DRHODT**2/DRHODP*XZ
      XGAMMA=CPOR/CVOR
      GAMMAE=XGAMMA/DRHODP
      RHOR=1./(10.**CAPU)
      TEST=(GAMMAE/GAM   *P/PREF*RHOR)
      IF(TEST.LE.0.) WRITE(6,1002) CAPX(KP),CAPU,XZ,CHORT,SOR ,LOGNE,DRH
     1ODT,DRHODP,CPOR ,CVOR ,XGAMMA,GAMMAE,AOAO
      AOAO=SQRT(TEST)
      WRITE(6,1002) CAPX(KP),CAPU,XZ,CHORT,SOR ,LOGNE,DRHODT,DRHODP,CPO
     1R,CVOR ,XGAMMA,GAMMAE,AOAO
      IF(NNN.EQ.10) GO TO 608
      GO TO 609
  608 WRITE(6,999)
      NNN=0
  609 NNN=NNN+1
      ABL(KP)=AOAO*AO
      SBL(KP)=SOR
      HBL(KP)=CHORT*T*8.31469E7/MU
   39 CONTINUE
      CALL INTER(PN,T,NCAPX,SBL,HBL,ABL,SOR4,KI)
   19 CONTINUE
      RETURN
      END
```

```
$IBFTC INTER   DECK
      SUBROUTINE INTER(PN,TM,N,SBL,HBL,ABL,SOR4,M)
      DIMENSION PN(30),SBL(30),HBL(30),ABL(30) ,
     1AM(30),HM(30)
      COMMON/BLOCK/HM,AM,M,P3(30)
      DO 5 I=1,N
    5 PN(I)=ALOG10(PN(I))
      NP=1
      CALL FTLUP(SOR4,P3(M),NP,N,SBL,PN)
      NP=-1
      CALL FTLUP(P3(M),HM(M),NP,N,PN,HBL)
      CALL FTLUP(P3(M),AM(M),NP,N,PN,ABL)
      DO 45 I=1,N
   45 PN(I)=10.**PN(I)
      P3(M)=10.**P3(M)
      RETURN
      END
```

```
$IBFTC INTEG   DECK
      SUBROUTINE INTEG(DU,U4)
      EXTERNAL FUNC
      DIMENSION AM(30),HM(30),DU(30)    ,SU(1,30)
      COMMON/BLOCK/HM,AM,M,P3(30)
      DO 1  I=1,M
    1 AM(I)=1./AM(I)
      DU(1)=U4
      DO 10 I=2,M
      NN=I
      CALL MGAUSS(HM(1),HM(I),NN,SU(1,I),FUNC,FOFX,1)
   10 DU(I)=U4-SU(1,I)/30.48
      RETURN
      END
```

```
$IBFTC PERNS   DECK
      SUBROUTINE PERNS(P1,T1,GAMMA,MU,R,P2,U2,NUMP)
      REAL MU
      DIMENSION P2(30),U2(30)
      GAMM=GAMMA-1.
      GAMP=GAMMA+1.
      SQGRT=SQRT(GAMMA*R*T1/MU)
      DO 10 I=1,NUMP
      U2(I)=SQGRT*(P2(I)/P1-1.)*SQRT((2./GAMMA)/(GAMP*P2(I)/P1+GAMM))
   10 U2(I)=U2(I)/30.48
      RETURN
      END
```

```
$IBFTC NORMAL  DECK
      SUBROUTINE NORMAL(P10,T10)
C
C                P-886.5
C            NORMAL SHOCK PROGRAM
C            PROGRAMMED FOR THE IBM 7094
C       YIELDING SOLUTIONS FOR FLOW PARAMETERS IN ARBITRARY GAS
C      MIXTURES IN THE FOLLOWING SITUATIONS-
C                    1. BEHIND NORMAL SHOCK
C
C
      DIMENSION YSTO(30),SHBL(8)
C
C     EQUILIBRIUM INPUT
      REAL MU
      INTEGER PUN,COMPUT,REAL,EXPO
      COMMON /BLOCK1/ICODE(30),F(30),CAPM(30),DHF0(30),L(30),G(30,30),
     1SMLE(30,30),CAPLAM(30,30),OMEG(5,30,30),A(10,30),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      COMMON PN(30),TM(30),NUMT,NCAPX,SOR4,U4,P4,T4,U3(30),
     1PUN,EXPO,REAL,COMPUT,P1,T1,P2(30),NUMP,USTO(30),U2(30)
      COMMON ISPEC(30),JMOL(10),M,N,BETA(5),NS,
     1AMC,NB,NBTA(5),MU,GAMMA,R,NAME(10)
C
C
C       SHOCK PROGRAM INPUT
C
C
C
      IF(NS.EQ.1) WRITE(6,4001) P10,T10
 4001 FORMAT(1H1,13H NORMAL SHOCK/4H P1=E15.7,2X,3HT1=E15.7)
      P10=P10*1.01325E6
      DO 100 IJ=1,NUMP
      CALL SLITET(2,KK)
      GO TO (44,45),KK
   44 CALL TAPE(N,ISPEC,M,JMOL)
   45 M=M
      US=USTO(IJ)
      AMC=0.
      DO 52 I=1,NB
      J=NBTA(I)
   52 AMC=AMC+BETA(I)*CAPM(J)
      A10=368.*SQRT(T10/AMC)
      AM10=US/A10
C
```

```
C      SET UP GUESS Y(I)
C
       IF(ISPEC(1).EQ.1)GO TO 48
       DO 46 I=1,N
   46  YSTO(I)=1.E-12
       GO TO 51
   48  YSTO(1)=0.
       DO 49 I=2,N
   49  YSTO(1)=YSTO(1)+A(M,I)*1.E-12
       YSTO(1)=-YSTO(1)
       DO 50 I=2,N
   50  YSTO(I)=1.E-12
   51  CONTINUE
       DO 3035 I=1,NB
       J=NBTA(I)
 3035  YSTO(J)=BETA(I)/AMC
       RHO10=P10/(T10/300.)*.040619*AMC
       TP=T10*(1.+.16*(1.5*AM10**2+1.)/AM10**2*(AM10**2-1.))
      1*(1.-.5*(US-5000.)/15000.)
       RHO2=RHO10*(4.*AM10**2)/(.5* AM10**2+2. )
C      CONVERSION
       RHO10=RHO10*1.E-3
       RHO2=RHO2*1.E-3
       US=US*30.48
       IF(T10.LE.800.) CALL SLITE(4)
       CALL ECOM(T10,P10,OOZ,HOZRT,H10,RHO10,YSTO,SOR)
C
C      STORE INITIAL P,T,RHO,AND U IN SHBL(1-4)
C
       SHBL(1)=P10
       SHBL(2)=T10
       SHBL(3)=RHO10
       SHBL(4)=US
       CALL SHOCK(TP,SHBL,H10,YSTO,RHO2,US)
C
C      UPON RETURN SHBL(5-8) CONTAINS P2,T2,RHO2,AND UF
C
       PPRINT=SHBL(5)/CONPRF
C
       UPRINT=SHBL(8)/30.48
C
       P2(IJ)=PPRINT
       U2(IJ)=UPRINT
       IF(NS.NE.1) GO TO 100
       WRITE(6,202) US,PPRINT,SHBL(7),OOZ,HOZRT,SOR,SHBL(6),AMC
```

```
202 FORMAT(//4H US=E15.7//9X,1HP,13X,3HRHO,14X,3H1/Z,14X,5HH/ZRT,
   X12X,3HS/R,
   114X,1HT,16X,2HM1//(7E17.8))
       WRITE(6,221)
221 FORMAT(//23H FINAL Y FROM ITERATION,4X,7HSPECIES//)
    WRITE(6,220) (YSTO(I),ICODE(I),I=1,N)
220 FORMAT(E17.8,10X,1A6)
100 CONTINUE
    P10=P10/1.01325E6
    RETURN
    END
```

```
$IBFTC TAPE    DECK
      SUBROUTINE TAPE(N,ISPEC,J,JMOL)                                   08967
C
      COMMON /BLOCK1/ICODE(30),F(30),CAPM(30),DHF0(30),L(30),G(30,30),
     1SMLE(30,30),CAPLAM(30,30),OMEG(5,30,30),A(10,30),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      DIMENSION BLOCK(150),LBLOCK(30),ISPEC(30),JMOL(10),
     1OBL(5,30)                                                         08967
      READ (9) (LBLOCK(I),I=1,30 )                                      08967
      DO 1 IC=1,N                                                       08967
      ISP=ISPEC(IC)                                                     08967
    1 ICODE(IC)=LBLOCK(ISP)                                             08967
C                                                                       08967
      READ (9) (BLOCK(I),I=1,30)                                        08967
      DO 2 IC=1,N                                                       08967
      ISP=ISPEC(IC)                                                     08967
    2 F(IC)=BLOCK(ISP)                                                  08967
C                                                                       08967
      READ (9) (BLOCK(I),I=1,30)                                        08967
      DO 3 IC=1,N                                                       08967
      ISP=ISPEC(IC)                                                     08967
    3 CAPM(IC)=BLOCK(ISP)                                               08967
C                                                                       08967
      READ(9)(BLOCK(I),I=1,30)
      DO 4 IC=1,N                                                       08967
      ISP=ISPEC(IC)                                                     08967
    4 DHF0(IC)=BLOCK(ISP)                                               08967
C                                                                       08967
      READ(9)(LBLOCK(I),I=1,30)                                         08967
      DO 5 IC=1,N                                                       08967
      ISP=ISPEC(IC)                                                     08967
    5 L(IC)=LBLOCK(ISP)                                                 08967
C                                                                       08967
      IC=1
      DO 6 I=1,30                                                       08967
      READ (9) (BLOCK(IL),IL=1,30)
      IF(ISPEC(IC)-I)6,55,6
   55 DO 56 LI=1,30                                                     08967
   56 G(LI,IC)=BLOCK(LI)
      IC=IC+1
    6 CONTINUE                                                          08967
C                                                                       08967
      IC=1
      DO 7 I=1,30                                                       08967
      READ (9) (BLOCK(IL),IL=1,30)                                      08967
      IF(ISPEC(IC)-I)7,65,7
   65 DO 66 LI=1,30                                                     08967
   66 SMLE(LI,IC)=BLOCK(LI)
      IC=IC+1
    7 CONTINUE                                                          08967
      IC=1
      DO 12 I=1,30
      READ (9) (BLOCK(IL),IL=1,30)                                      08967
      IF(ISPEC(IC)-I)12,13,12
   13 DO 125 LI=1,30                                                    08967
  125 CAPLAM(LI,IC)=BLOCK(LI)
      IC=IC+1
   12 CONTINUE                                                          08967
C                                                                       08967
      IIC=1
      DO 8 I=1,30                                                       08967
      READ(9) ((OBL(IC,IL),IC=1,5),IL=1,30)
      IF(ISPEC(IIC)-I)8,75,8
   75 DO 76 LI=1,30
      DO 76 IC=1,5                                                      08967
   76 OMEG(IC,LI,IIC)=OBL(IC,LI)
      IIC=IIC+1
    8 CONTINUE
C                                                                       08967
      IC=1
      DO 10 I=1,30                                                      08967
      READ(9)(BLOCK(IJ),IJ=1,10)                                        08967
      IF(ISPEC(IC)-I)10,85,10
   85 DO 9 IJ=1,J                                                       08967
      IJM=JMOL(IJ)                                                      08967
    9 A(IJ,IC)=BLOCK(IJM)
      IC=IC+1
   10 CONTINUE                                                          08967
C                                                                       08967
      CONR=8.3146938E7
      CONPRF=1.01325E6
      CONNO=6.02322E23
      CONH=6.62517E-27
      CONK=1.38044E-16
      PI=3.14159                                                        08967
      NIT=300
      EPS1=1.E-7
      EPS2=.01
      IF(ISPEC(N)-28)14,15,14
   14 IC1=1                                                             08967
```

```
$IBFTC SHOCK   DECK
      SUBROUTINE SHOCK(TGUESS,BLOCK,H10,YSTO,RHO2,US)
C
C     THIS SUBROUTINE USES A ONE-DIMENSIONAL NEWTON-RAPHSON ITERATION
C     SCHEME TO FIND TEMPERATURE AND PRESSURE AT EQUILIBRIUM BEHIND
C     INCIDENT SHOCK.  IT WILL CALL SUBROUTINE ECOM TO COMPUTE THE
C     EQUILIBRIUM PROPERTIES.
      DIMENSION YSTO(30)
      DIMENSION T(2),H(2),BLOCK(8)
C
C
C     LET RHO2 = FIRST RHO
C
      VEL1(AA)=C*D/AA
      PRES1(AA,BB)=B+C*D**2-AA*BB**2
      ENTH1(AA)=H10+(D**2)/2.-(AA**2)/2.
      DELT=10.
      IT=3
      EPS5=1.E-5
      NCOUNT=1
      B=BLOCK(1)
      C=BLOCK(3)
      D=BLOCK(4)
      U2=VEL1(RHO2)
      P2=PRES1(RHO2,U2)
      H2=ENTH1(U2)
C
C     COMPUTE FIRST POINT
C
      ITT=IT
    7 T(1)=TGUESS
      CALL ECOM(T(1),P2,OOZ,HOZRT,H(1),RHO,YSTO,SOR)
C
C     COMPUTE SECOND POINT
C
      T(2)=T(1)+DELT
      CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO,YSTO,SOR)
      S=(H(2)-H(1))/(T(2)-T(1))
      T(1)=T(2)
C
C     TEMPERATURE FROM FIRST ITERATION
C
      T(2)=T(2)+(H2-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,8
    8 CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO,YSTO,SOR)
C
C     S IS SLOPE    (H2-H1)/(T2-T1)
C
   85 S=(H(2)-H(1))/(T(2)-T(1))
C     T3
      T(1)=T(2)
C
C     TEMPERATURE FROM SECOND ITERATION
C
      T(2)=T(2)+(H2-H(2))/S
      H(1)=H(2)
      IF(T(2))25,25,9
    9 CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO,YSTO,SOR)
C
C     IF ITT IS GREATER THAN 2, ITERATE AGAIN ON TEMPERATURE WITH
C          FIRST PRESSURE
C
      IF(ITT-2)10,10,11
   10 SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
   11 ITT=ITT-1
      GO TO 85
C
C
C     TEST RHO FOR CONVERGENCE
C
   12 IF(ABS((RHO-RHO2)/RHO2)-EPS5)20,20,13
C
C     NON-CONVERGENCE-
C
C     COMPUTE NEW PRESSURE AND CONTINUE ITERATION ON TEMPERATURE AND
C          PRESSURE UNTIL RHO CONVERGES
C
   13 RHO2=RHO
      U2=VEL1(RHO2)
      P2=PRES1(RHO2,U2)
      H2=ENTH1(U2)
      NCOUNT=NCOUNT+1
      T(1)=TLAST
   14 CALL ECOM(T(1),P2,OOZ,HOZRT,H(1),RHO,YSTO,SOR)
  145 S=SLAST
   15 T(2)=T(1)+(H2-H(1))/S
```

```
      CALL ECOM(T(2),P2,OOZ,HOZRT,H(2),RHO,YSTO,SOR)
      SLAST=(H(2)-H(1))/(T(2)-T(1))
      TLAST=T(2)
      GO TO 12
C
C     CONVERGENCE -  STORE OUTPUT
C
   20 U2=VEL1(RHO)
      UF=US-U2
      RHO=RHO*1.E3
      BLOCK(5)=P2
      BLOCK(6)=TLAST
      BLOCK(7)=RHO
      BLOCK(8)=UF
      RETURN
C
C     TEMPERATURE ESTIMATE TOO HIGH      -  ADJUST
C
   25 TGUESS=(TGUESS-T10)/2.
      GO TO 7
      END
```

APPENDIX

```
$IBFTC ECOM    DECK
      SUBROUTINE ECOM(T,PSTO,OOZ,HOZRT,H,RHO,YSTO,SOR)
C
C     SUBROUTINE WHICH, GIVEN A TEMPERATURE AND PRESSURE, COMPUTES
C     THE THERMODYNAMIC EQUILIBRIUM PROPERTIES OF A GAS DESCRIBED BY
C     THE INPUT.
C
      REAL MU
      INTEGER PUN,COMPUT,REAL,EXPO
      DIMENSION SMALE(30,30),X(30),YSTO(30)
      DIMENSION E(30),Y(30;,Q(30),CAPFI(30),R(10,10),B(10),
     3TEMPS(10),BSUM(11,1),ABLOCK(11,11),PTEMP(30),ZETA(30),
     4ZETAPR(30),ALAM(30),
     5IPIVOT(11),DQINT(30),QINT(30,30)
C
      COMMON /BLOCK1/ICODE(30),F(30),CAPM(30),DHFO(30),L(30),G(30,30),
     1SMLE(30,30),CAPLAM(30,30),OMEG(5,30,30),A(10,30),CONR,CONPRF,
     2CONNO,CONH,CONK,PI,EPS1,NIT,EPS2,IC1
      COMMON PN(30),TM(30),NUMT,NCAPX,SOR4,U4,P4,T4,U3(30),
     1PUN,EXPO,REAL,COMPUT,P1,T1,P2(30),NUMP,USTO(30),U2(30)
      COMMON ISPEC(30),JMOL(10),M,N,BETA(5),NS,
     1AMC,NB,NBTA(5),MU,GAMMA,R,NAME(10)
C
      EQUIVALENCE(SMLE(1,1),SMALE(1,1)),(ICODE(1),CODE(1))
C
      PI=3.14159
      C=2.99793E10
      NCOUNT=0
      LTEST=LTEST
      N2=N
      DO 5 I=1,N
    5 Y(I)=YSTO(I)
      P=PSTO
   34 TK=CONK*T
      RT=CONR*T
  346 YBAR=0.0
      DO 347 I=1,N
  347 YBAR=YBAR+Y(I)
      DO 40 I=1,N
      TEMP1=0
      LEND=L(I)
      DO 37 L1=1,LEND
      IF(F(I))31,35,31
   31 PROD=1.
      DO 33 IC=1,IC1
      IF(OMEG(IC,L1,I))32,33,32
   32 PROD=PROD*(1.-EXP(-CONH*C*OMEG(IC,L1,I)/TK))
   33 CONTINUE
      PART=(T/(CAPLAM(L1,I)*PROD))**F(I)
      GO TO 36
   35 PART=1.
   36 QINT(L1,I)=PART*G(L1,I)*EXP(-CONH*C*SMALE(L1,I)/TK)
   37 TEMP1=TEMP1+QINT(L1,I)
      Q(I)=(SQRT(2.*PI/CONH*TK/(CONH*CONNO)*CAPM(I))**3)*TK/CONPRF*TEMP1
      IF(Y(I))38,38,39
   38 CAPFI(I)=0
      GO TO 40
   39 CAPFI(I)=Y(I)*(ALOG(P/CONPRF)+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
   40 CONTINUE
      CALL SLITET(4,JJ)
      GO TO (95,396),JJ
  396 DO 50 J=1,M
      DO 50 K=1,M
      R(K,J)=0.0
      B(J)=0.0
      DO 50 I=1,N
      B(J)=B(J)+A(J,I)*Y(I)
   50 R(K,J)=R(K,J)+A(J,I)*A(K,I)*Y(I)
C
C     SET UP MATRIX FOR SOLUTION OF EQUATIONS
C
      DO 60 J=1,M
      TEMPS(J)=0.0
      DO 55 I=1,N
   55 TEMPS(J)=TEMPS(J)+A(J,I)*CAPFI(I)
      BSUM(J,1)=B(J)+TEMPS(J)
C
C     CONSTANT TERMS IN BSUM BLOCK
C
      DO 56 K=1,M
      K1=K+1
   56 ABLOCK(J,K1)=R(K,J)
C
C     PI TERMS IN ABLOCK IN COLUMNS 2 THROUGH N+1
C
   60 ABLOCK(J,1)=B(J)
C
C     (X/Y) TERMS IN FIRST COLUMN
C
```

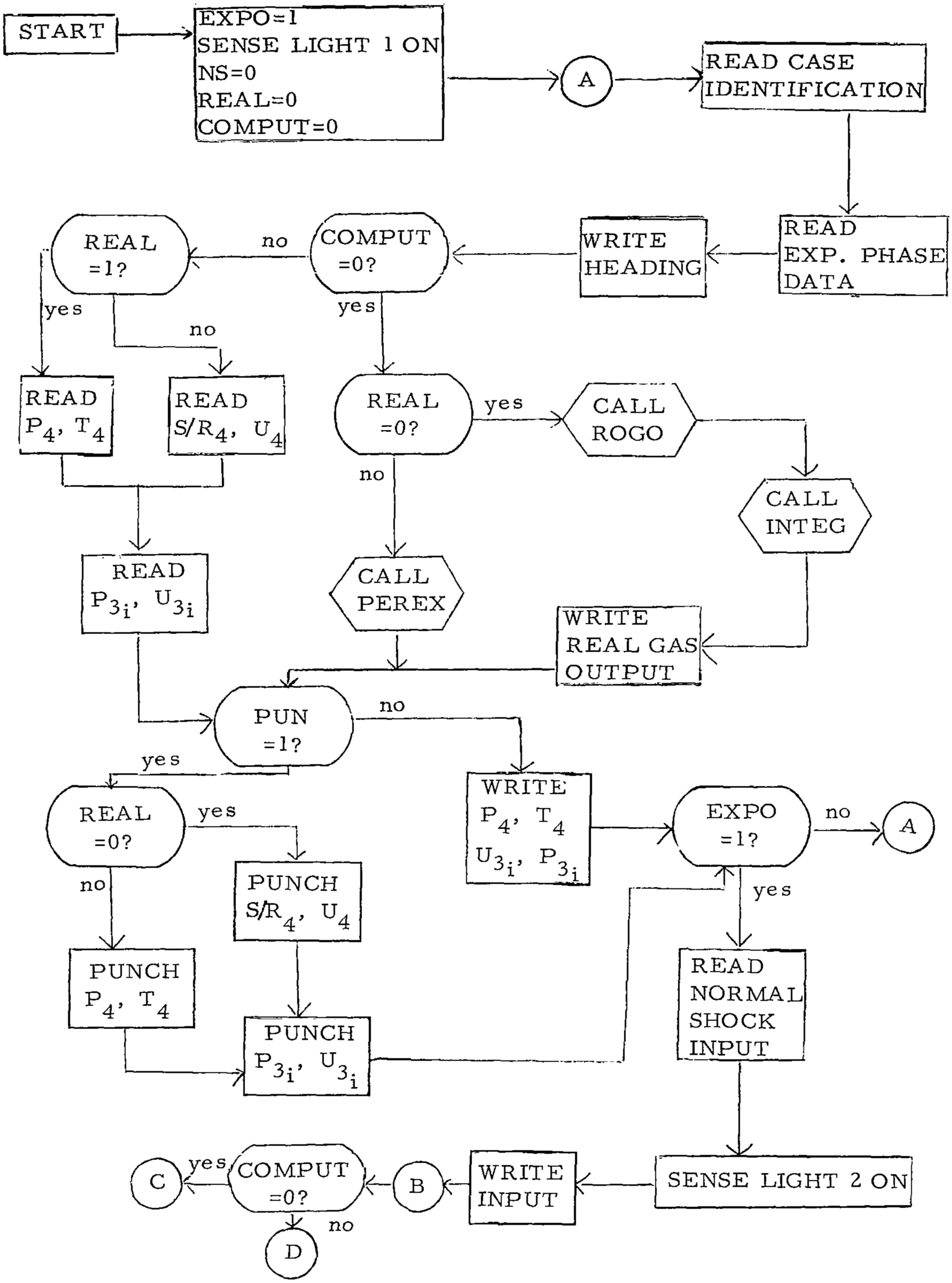
```
      M1=M+1
      ABLOCK(M1,1)=0.0
      DO 61 K=1,M1
      K1=K+1
   61 ABLOCK(M1,K1)=B(K)
      BSUM(M1,1)=0.0
      DO 62 I=1,N
   62 BSUM(M1,1)=BSUM(M1,1)+CAPFI(I)
C
C     MATINV EXPECTS AN M+1 BY M+1 MATRIX
C
      CALL SIMEQ(ABLOCK(1,1),M1,BSUM(1,1),1,DETERM,IPIVOT,11,0)
C
C     RETURN WITH ANSWERS IN BSUM
C
      ZETAP=BSUM(1,1)*YBAR
      ZERO=0.
      NEG=0.0
      DO 70 I=1,N
      PTEMP(I)=0.0
      DO 65 J=1,M
      J1=J+1
   65 PTEMP(I)=PTEMP(I)+BSUM(J1,1)*A(J,I)*Y(I)
      ZETA(I)=-CAPFI(I)+Y(I)*BSUM(1,1)+PTEMP(I)
C
C     TEST FOR NEGATIVE OR ZERO ZETA
C
   68 IF(ZETA(I))69,695,70
   69 PIECE=-Y(I)/(ZETA(I)-Y(I))
      IF(PIECE)691,692,691
  691 NEG=NEG+1
      ALAM(NEG)=PIECE
      GO TO 70
  692 Y(I)=0
      ZERO=1.
      GO TO 70
  695 IF(Y(I))69,70,69
   70 CONTINUE
C
C     FIND GREATEST NEGATIVE ZETA-Y
C
      IF(ZERO)700,700,698
  698 IF(NCOUNT-NIT)699,100,100
  699 NCOUNT=NCOUNT+1
      GO TC 346
  700 IF(NEG-1)78,71,73
   71 ALAMPR=.999999*ALAM(1)
      GO TO 745
   73 ARG1=ALAM(1)
      DO 74 I=2,NEG
   72 ARG2=ALAM(I)
      ARG1=AMIN1(ARG1,ARG2)
   74 CONTINUE
      ALAMPR=.999999*ARG1
  745 IIC=0
   75 ZETAP=0
      DO 76 I=1,N
      ZETAPR(I)=Y(I)+ALAMPR*(ZETA(I)-Y(I))
   76 ZETAP=ZETAP+ZETAPR(I)
      DLAM=0
      DO 77 I=1,N
      IF(ZETAPR(I))77,77,765
  765 DLAM=DLAM+(ZETA(I)-Y(I))*(ALOG(P/CONPRF)-ALOG(Q(I))+DHFO(I)/RT+ALO
     1G(ZETAPR(I)/ZETAP))
   77 CONTINUE
      IF(DLAM)81,81,80
   80 IF(IIC-3)805,81,81
  805 IIC=IIC+1
      ALAMPR=ALAMPR*.9
      GO TO 75
   78 ALAMPR=1.
      GO TO 745
C
C     CONVERGENCE TEST FOR Y(I)S
C
   81 IF(ALAMPR-.50)83,815,815
  815 DO 82 I=1,N
      IF(ZETAPR(I))813,816,813
  813 REL=Y(I)-ZETAPR(I)
      IF(ABS(REL)-EPS1)818,818,83
  818 REL=ZETAPR(I)/Y(I)-1.
      IF(ABS(REL)-EPS2)82,82,83
  816 IF(Y(I))817,82,817
  817 GO TO 83
   82 CONTINUE
C
C     Y(I)S CONVERGE
C
      DO 800 I=1,N
  800 Y(I)=ZETAPR(I)
```

```
      GO TO 95
C
C     NON-CONVERGENCE OF Y(I)S
C
   83 NCOUNT=NCOUNT+1
      IF(NCOUNT-NIT)84,100,100
   84 DO 85 I=1,N
   85 Y(I)=ZETAPR(I)
C
C     REPEAT WITH NEW Y(I)S AND NO. OF ITERATIONS LESS THAN NIT
C
      GO TO 346
   95 DO 201  I=1,N
  201 X(I)=Y(I)*CAPM(I)
      YBAR=0.0
      CAPMI=0
      DO 2026 I=1,N
      YBAR=YBAR+Y(I)
 2026 CAPMI=CAPMI+X(I)/CAPM(I)
      CAPMI=1.0/CAPMI
      Z=AMC/CAPMI
      ESUM=0
      DO 2029 I=1,N
      QSUM=0
      DQINT(I)=0
      LEND=L(I)
      DO 2028 L1=1,LEND
      SUM=0
      DO 2027 IC=1,IC1
      HOOTK=CONH*C*OMEG(IC,L1,I)/TK
      IF(OMEG(IC,L1,I))2000,2027,2000
 2000 SUM=SUM+HOOTK/(EXP(HOOTK)-1.)
 2027 CONTINUE
      DQINT(I)=DQINT(I)+QINT(L1,I)*(F(I)/T*(1.+SUM)+SMALE(L1,I)*CONH*C
     1/(TK*T))
 2028 QSUM=QSUM+QINT(L1,I)
      E(I)=1./CAPM(I)*(1.5*RT+RT*T/QSUM*DQINT(I)+DHFO(I))
 2029 ESUM=ESUM+X(I)*E(I)
      HOZRT=CAPMI*ESUM/RT+1.0
      H=HOZRT*CONR*T*Z/AMC
      TK=T*CONK
      FSUM=0
      DO 2040 I=1,N
 2033 IF(Y(I))2034,2034,2035
 2034 CAPFI(I)=0
```

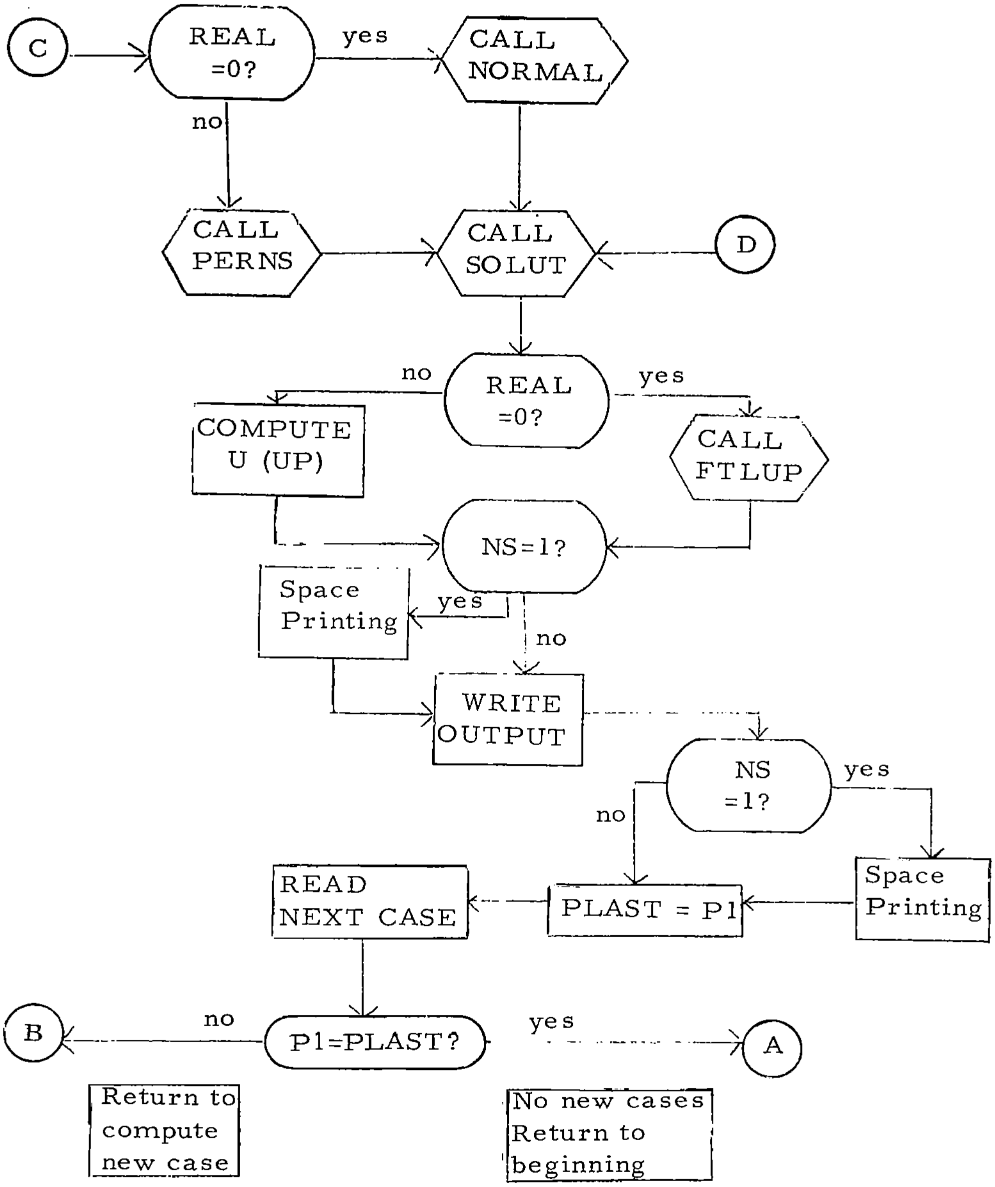
```
      GO TO 2040
 2035 CAPFI(I)=Y(I)*(ALOG(P/CONPRF)+ALOG(Y(I)/YBAR)-ALOG(Q(I))+DHFO(I)
     1/RT)
 2040 FSUM=FSUM+CAPFI(I)
      SOZR=HOZRT-CAPMI*FSUM
      SOR=SOZR*Z
      RHO=P*CAPMI/RT
      U=CAPX+.43429*ALOG(273.16/(Z*T))
      OOZ=1.0/Z
      DO 300 I=1.N
      YSTO(I)=Y(I)
  300 X(I)=X(I)*CAPMI/CAPM(I)
      RETURN
  100 WRITE(6.5000)
 5000 FORMAT(1H0.25H THIS CASE NON-CONVERGENT)
      CALL EXIT
      END
```

```
$IBFTC FOFX     DECK
      SUBROUTINE FUNC(DUM,FOFX)
      COMMON/BLOCK/HM,AM,M ,P3(30)
      DIMENSION HM(30),AM(30)
      CALL FTLUP(DUM,AA,-2,M,HM,AM)
      FOFX=AA
      RETURN
      END
```

```
$IBFTC SOLUT   DECK
      SUBROUTINE SOLUT(U3,P3,U2,P2,M,N,UR,P)
      DIMENSION U3(30),P3(30),U2(30),P2(30),U(2)
      FUNCD(PP,UU,R)=PP-UU*R
      FUNAB(P,PP,U,UU)=(P-PP)/(U-UU)
C
C     USE END POINTS FOR FIRST INTERSECTION
C
      MR=1
      NR=1
      IF(P2(1).GT.P2(2)) NR=-NR
      IF(P3(1).GT.P3(2)) MR=-MR
      P31=P3(1)
      P32=P3(M)
      P21=P2(1)
      P22=P2(N)
      U21=U2(1)
      U22=U2(N)
      U31=U3(1)
      U32=U3(M)
    5 AA=FUNAB(P22,P21,U22,U21)
      BB=FUNAB(P32,P31,U32,U31)
      CC=FUNCD(P21,U21,AA)
      DD=FUNCD(P31,U31,BB)
      UR=(CC-DD)/(BB-AA)
      PR=CC+UR*AA
      CALL FTLUP(PR,U(1),NR,N,P2,U2)
      CALL FTLUP(PR,U(2) ,MR,M,P3,U3)
      IF(ABS((U(1)-U(2))/U(1))-.0001)12,12,10
   10 P31=P32
      P32=PR
      P21=P22
      P22=PR
      U31=U32
      U32=U(2)
      U21=U22
      U22=U(1)
      GO TO 5
   12 P=PR
      RETURN
      END
```


START
EXPO=1
SENSE LIGHT 1 ON
NS=0
REAL=0
COMPUT=0
A
READ CASE IDENTIFICATION
READ EXP. PHASE DATA
WRITE HEADING
COMPUT =0?
no
yes
REAL =1?
yes
no
READ P_4, T_4
READ S/R_4, U_4
REAL =0?
yes
no
CALL ROGO
CALL INTEG
CALL PEREX
WRITE REAL GAS OUTPUT
READ P_{3_i}, U_{3_i}
PUN =1?
no
yes
WRITE P_4, T_4 U_{3_i}, P_{3_i}
EXPO =1?
no
A
yes
REAL =0?
yes
no
PUNCH S/R_4, U_4
PUNCH P_4, T_4
PUNCH P_{3_i}, U_{3_i}
READ NORMAL SHOCK INPUT
SENSE LIGHT 2 ON
WRITE INPUT
B
COMPUT =0?
yes
C
no
D

APPENDIX


C
REAL =0?
yes
CALL NORMAL
no
CALL PERNS
CALL SOLUT
D
no
REAL =0?
yes
COMPUTE U (UP)
CALL FTLUP
NS=1?
Space Printing
yes
no
WRITE OUTPUT
NS =1?
yes
no
Space Printing
READ NEXT CASE
PLAST = P1
B
no
P1=PLAST?
yes
A
Return to compute new case
No new cases Return to beginning

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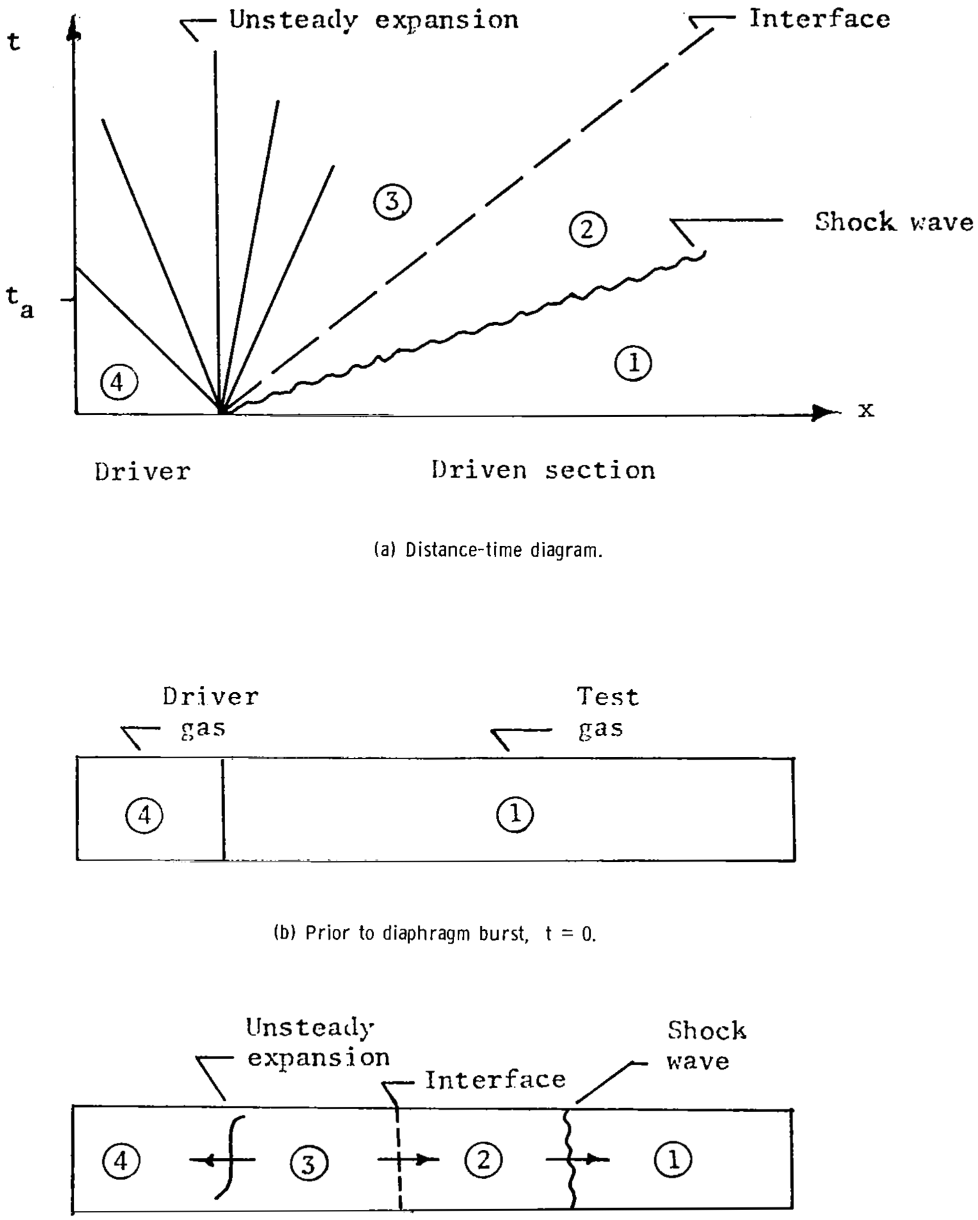

(a) Distance-time diagram.

(b) Prior to diaphragm burst, t = 0.

(c) After diaphragm burst, $t = t_a$.

Figure 1.- Operating sequence of a simple shock tube.

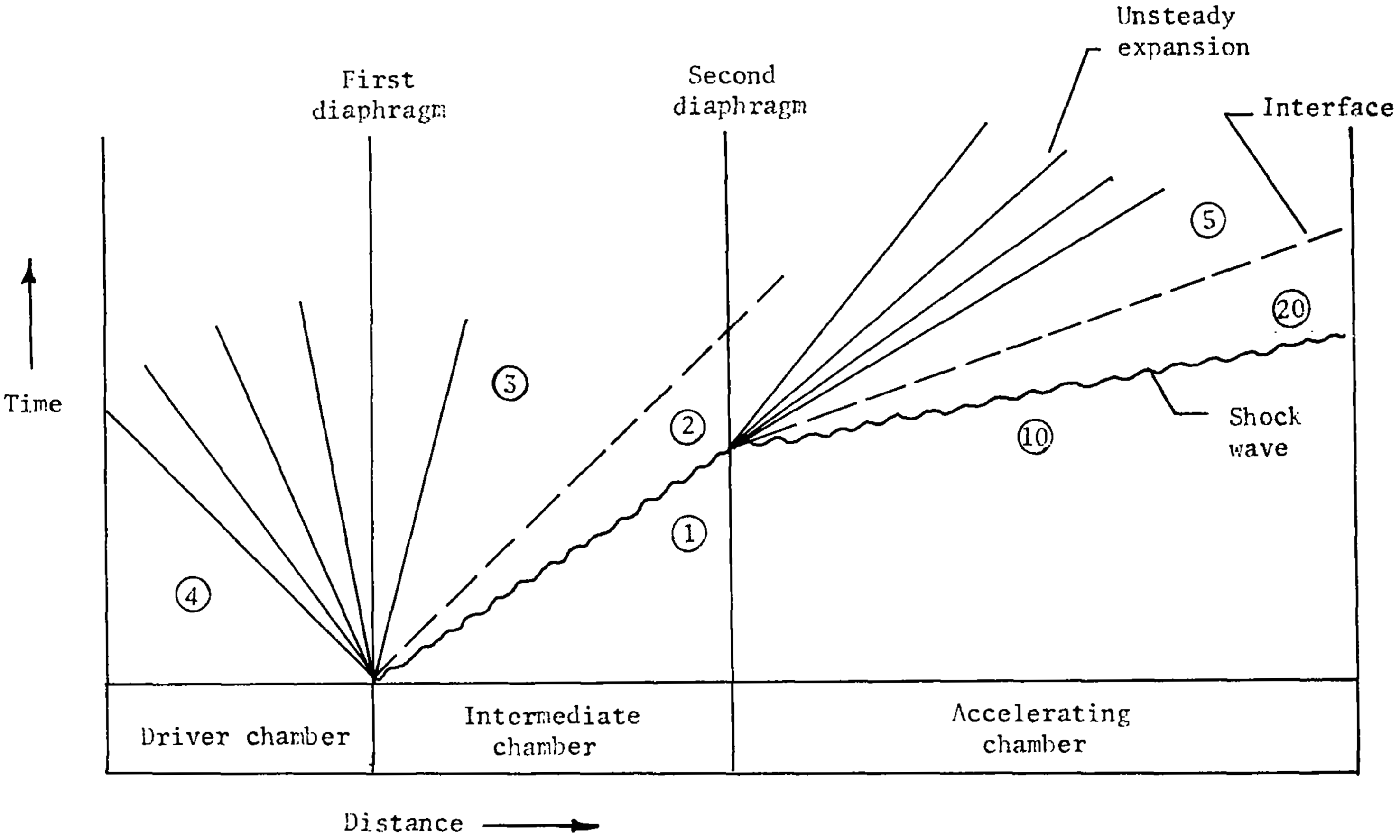

Figure 2.- Schematic diagram of expansion tube flow cycle.

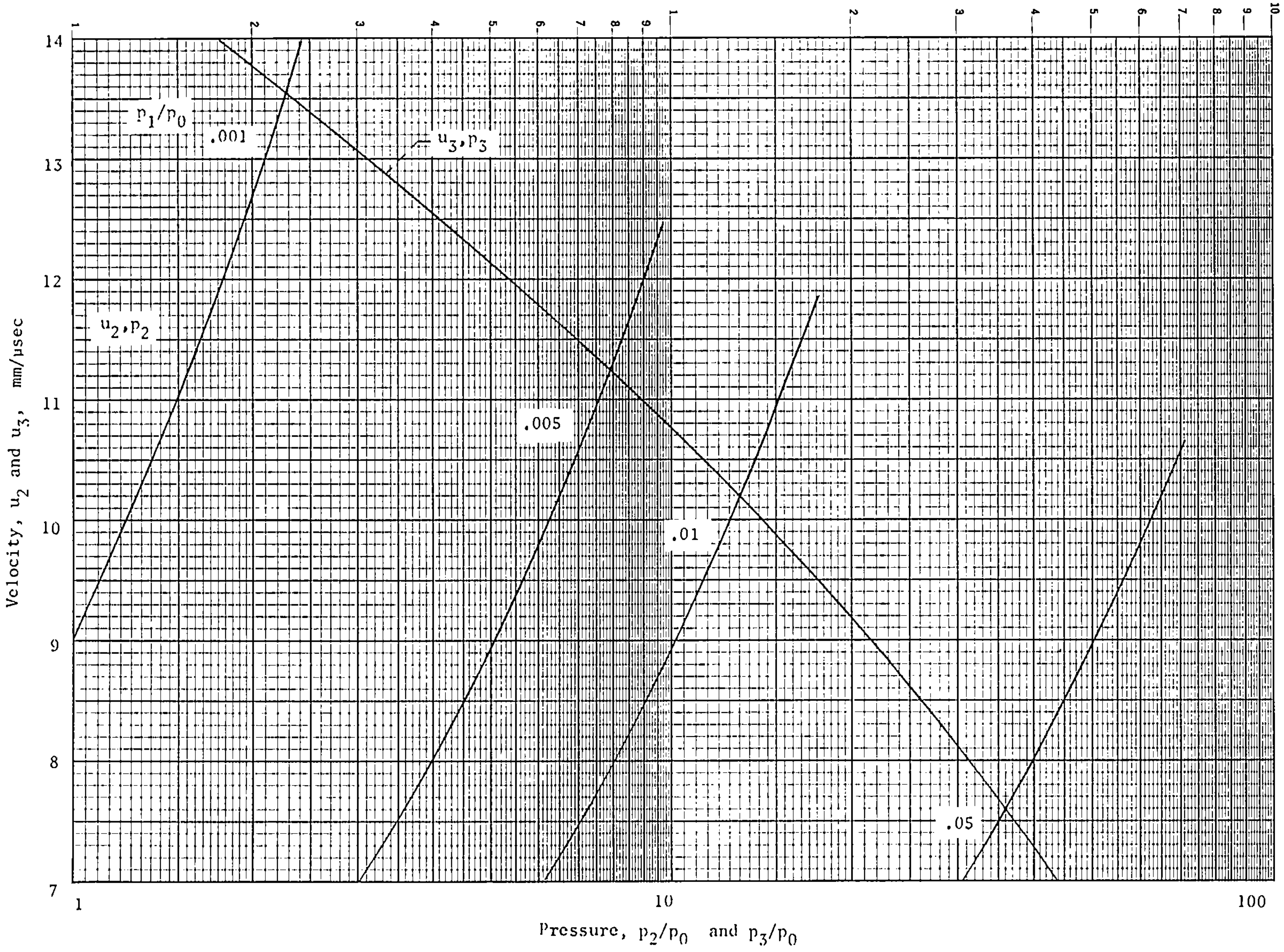

Figure 3.- Velocity u_3 as a function of pressure p_3 for real gas isentropic expansion of helium for $p_4/p_0 = 315$ and $T_4 = 15\ 000^{\circ}$ K; velocity u_2 as a function of pressure p_2 for incident normal shock in air.

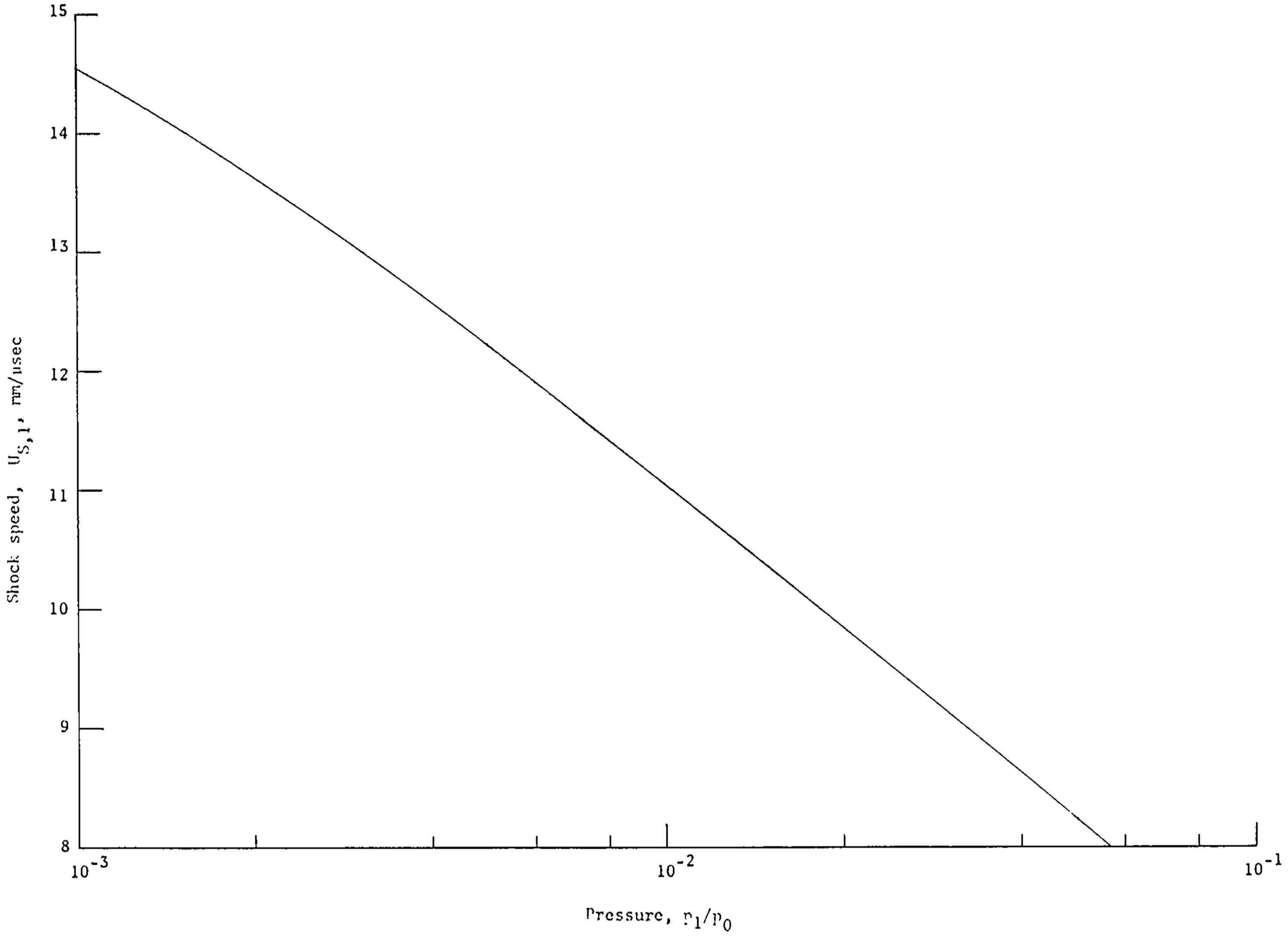

Figure 4.- Incident shock speed in air as a function of p_1/p_0 for initial helium driver conditions of $p_4/p_0 = 315$ and $T_4 = 15\ 000^\circ$ K.

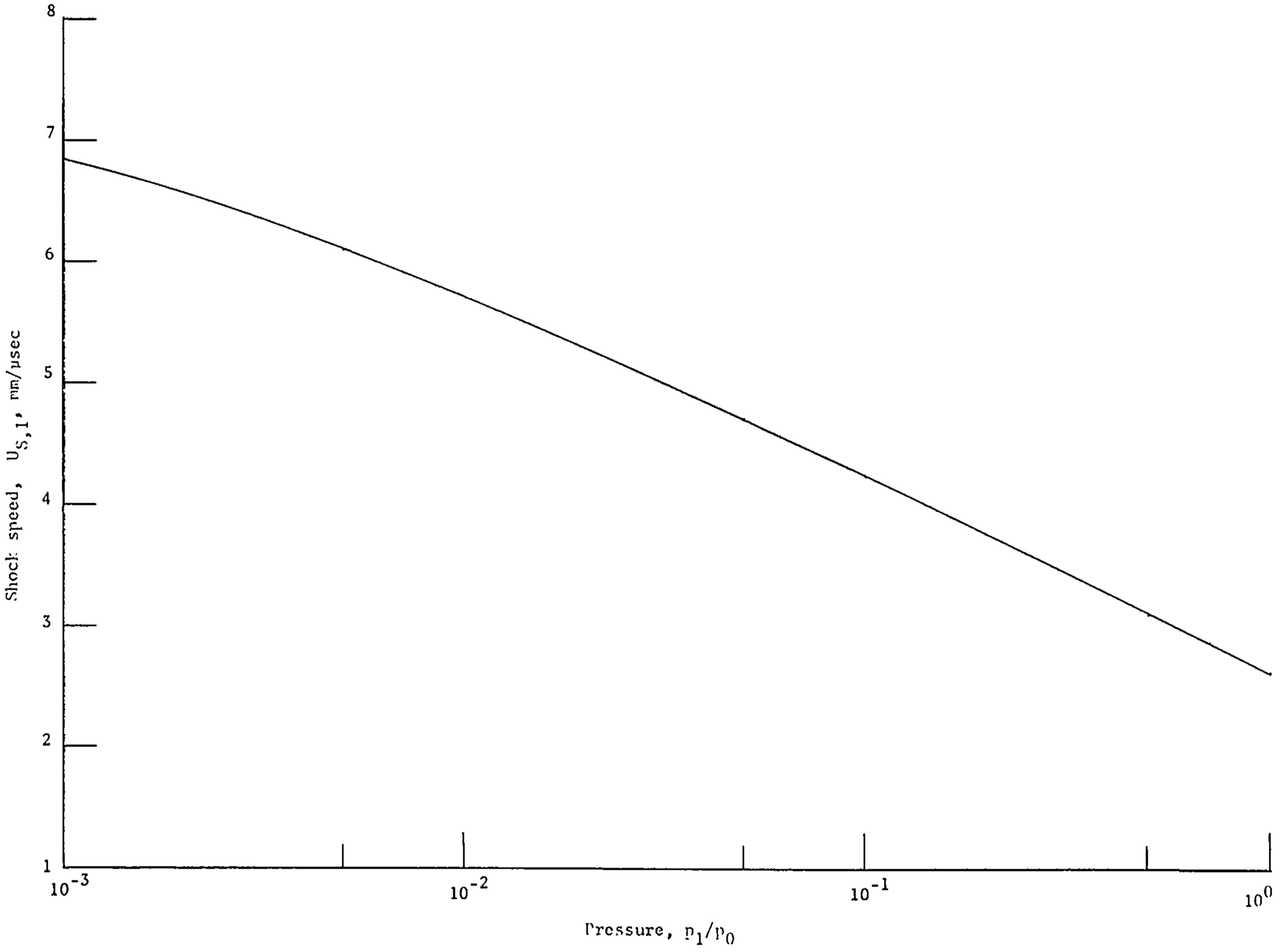

Figure 5.- Shock speed as a function of initial air pressure for helium driver conditions of $p_4/p_0 = 300$ and $T_4 = 2500^{\circ}$ K.

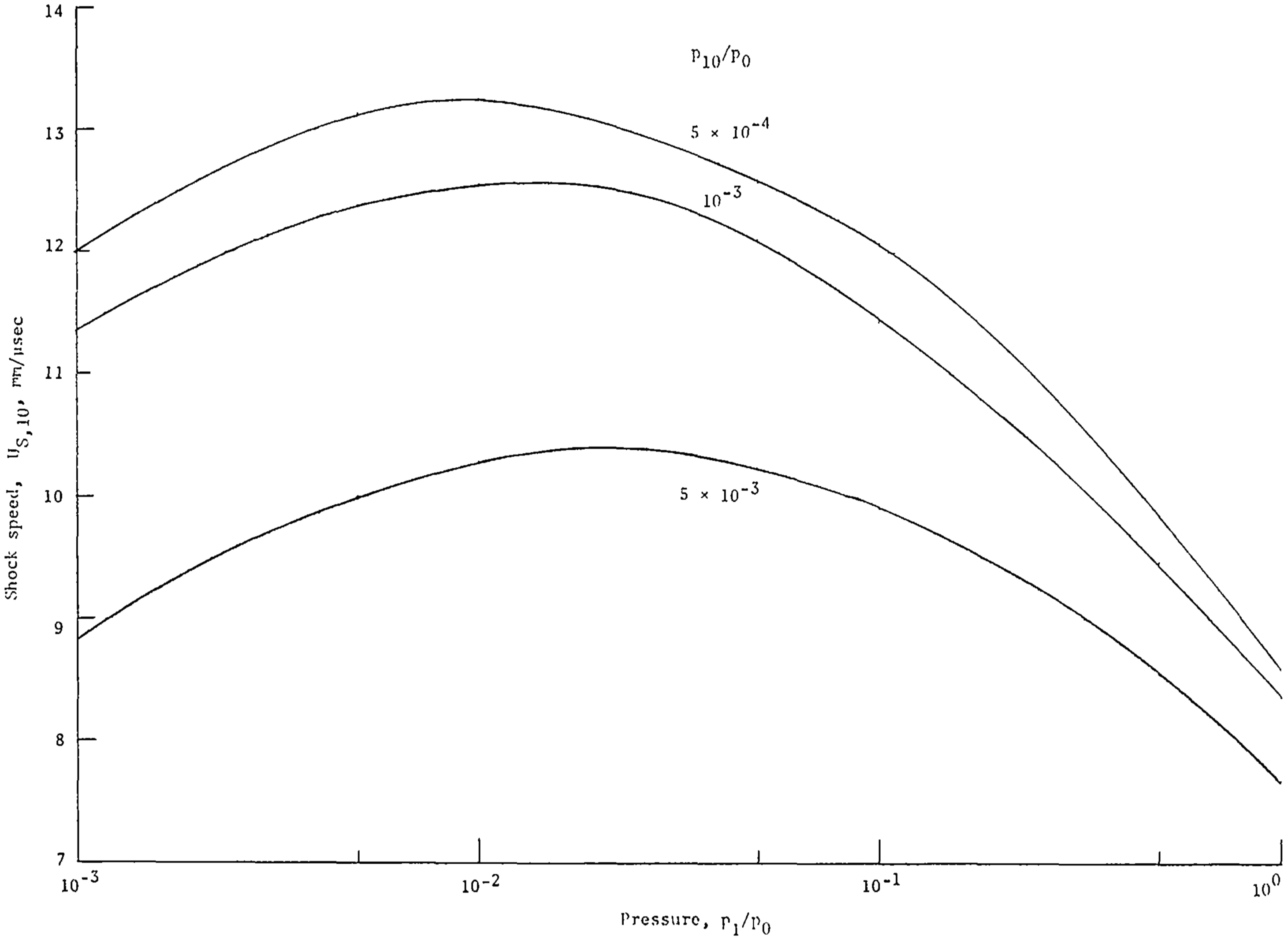

Figure 6.- Shock speed as a function of p_1/p_0 for helium driver conditions of $p_4/p_0 = 300$ and $T_4 = 2500^0$ K.

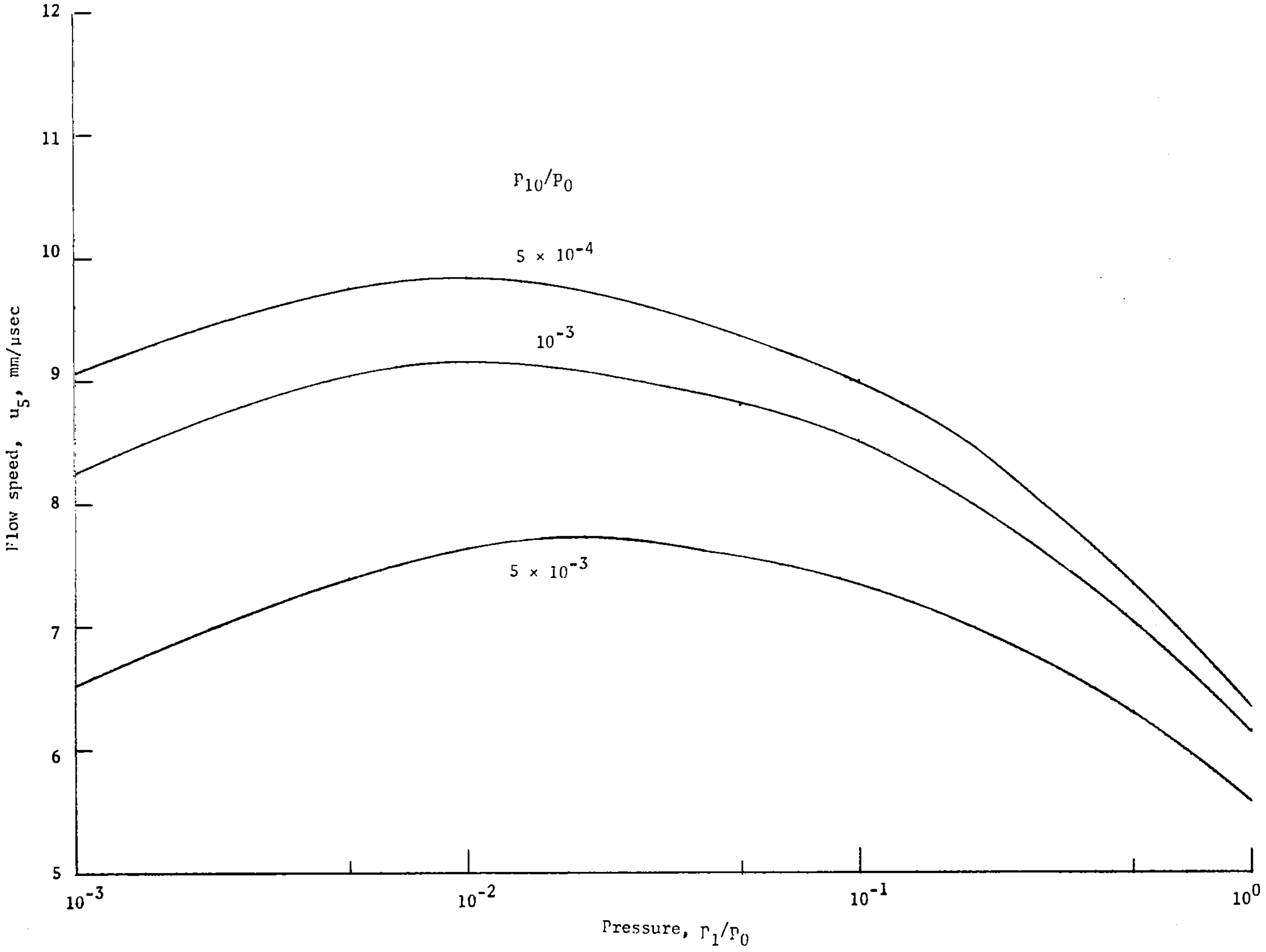

Figure 7.- Expansion tube test gas speed as a function of p_1/p_0 for helium driver conditions of $p_4/p_0 = 300$ and $T_4 = 2500^0$ K.

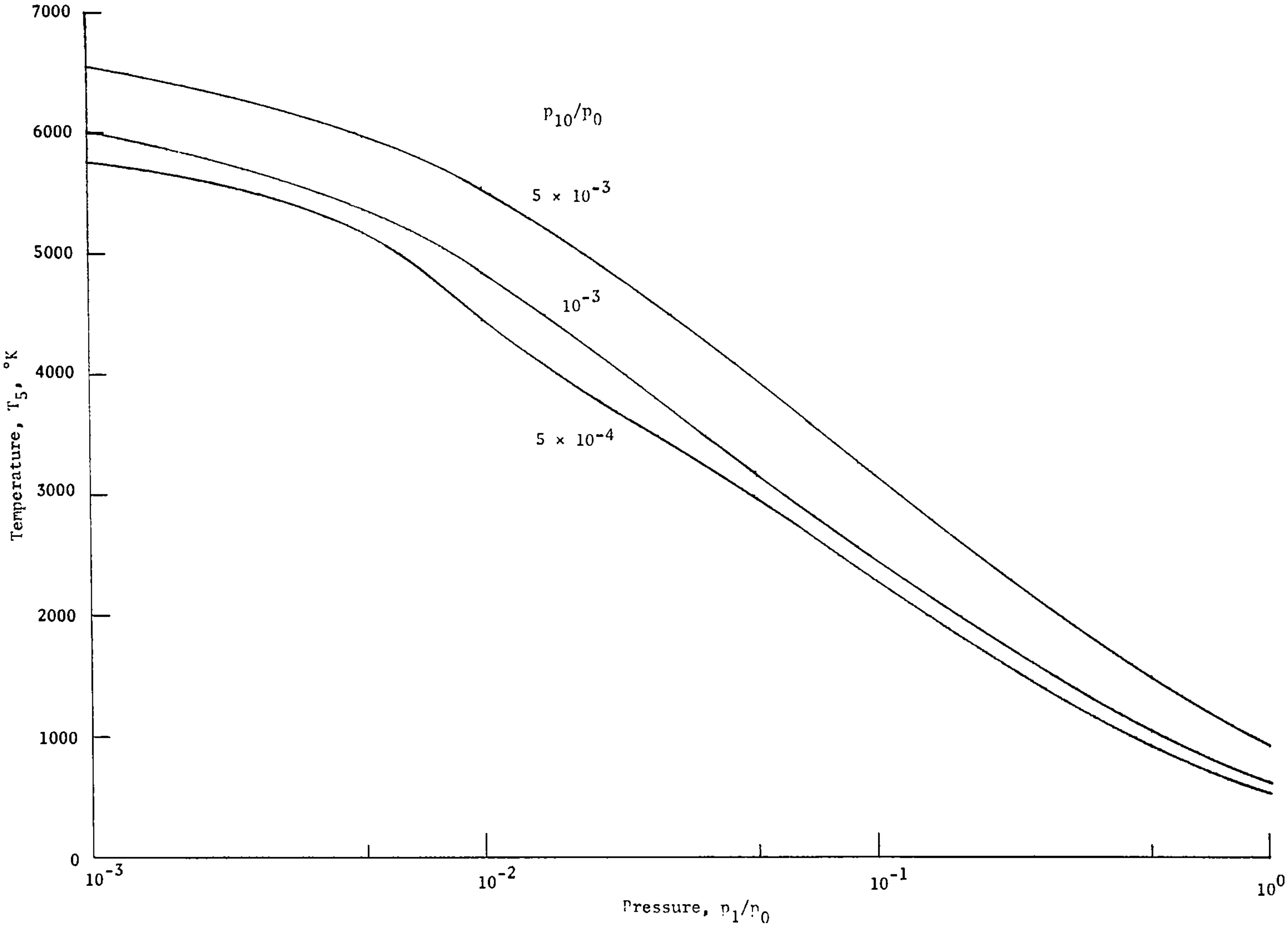

Figure 8.- Expansion tube test gas temperature as a function of initial air pressure for helium driver conditions of $p_4/p_0 = 300$ and $T_4 = 2500^{\circ}$ K.

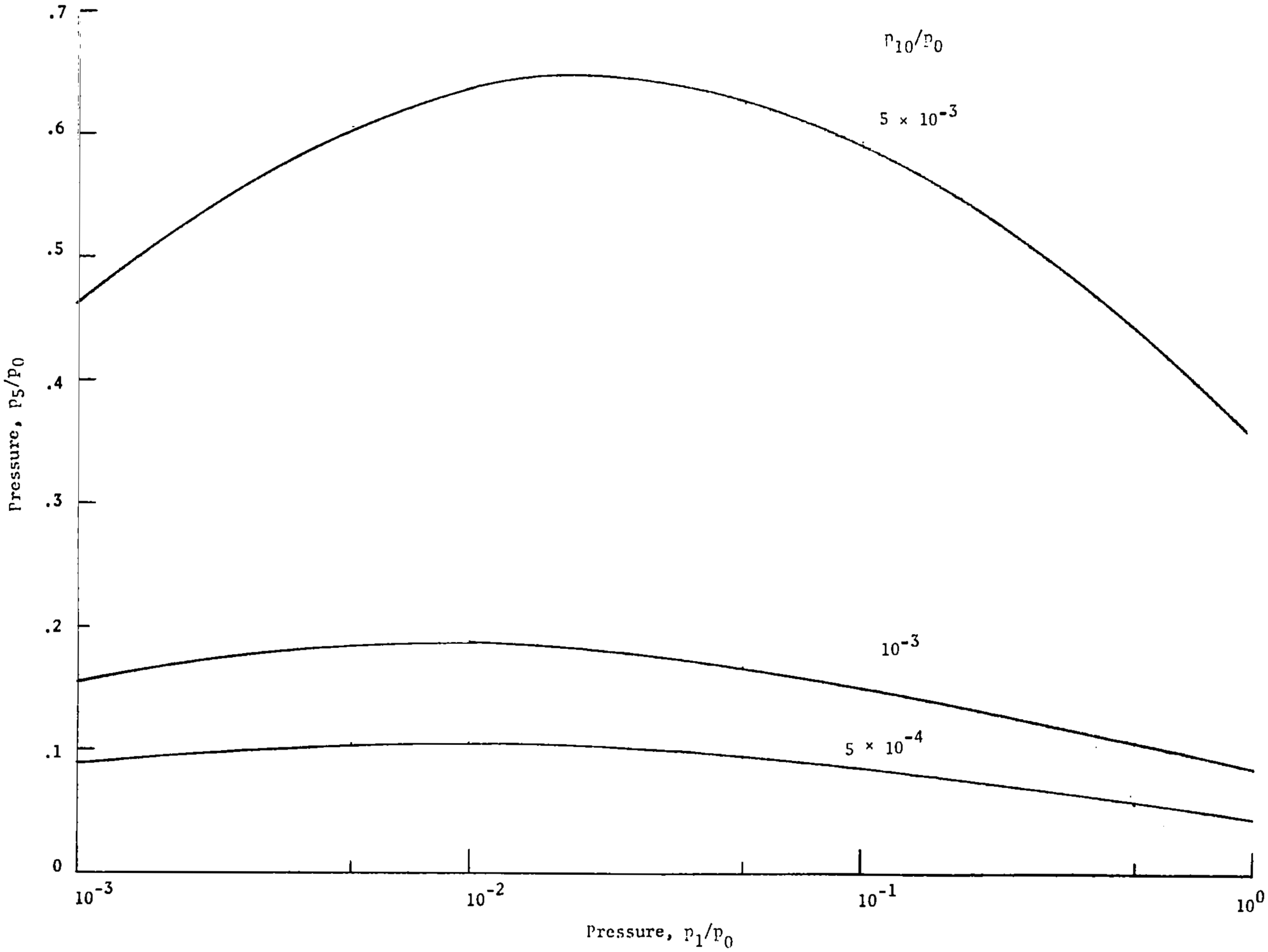

Figure 9.- Expansion tube test gas pressure as a function of initial air pressure for helium driver conditions of $p_4/p_0 = 300$ and $T_4 = 2500^0$ K.

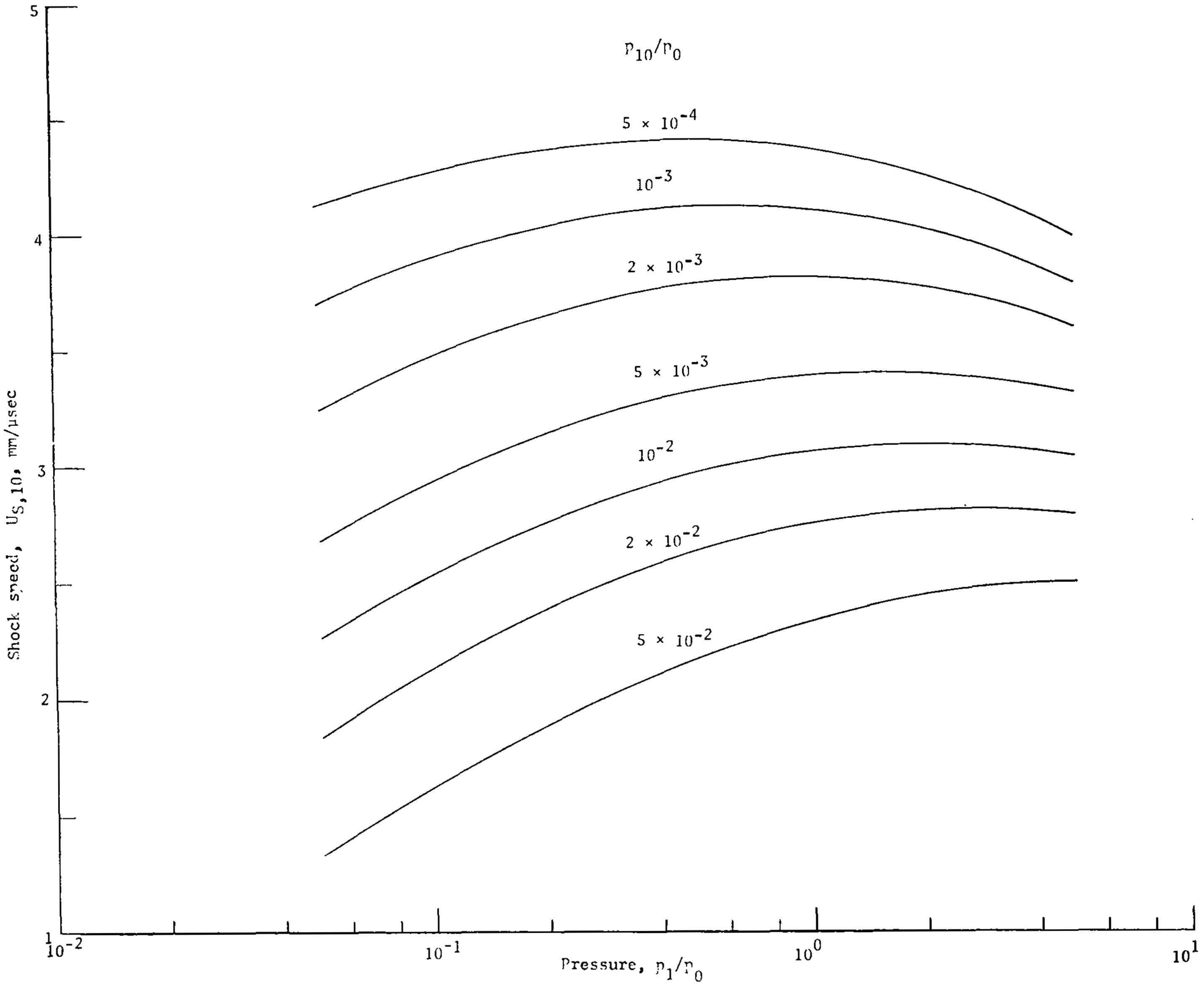

Figure 10.- Test gas shock speed as a function of buffer gas pressure for test gas of 90 percent N_2 and 10 percent CO_2 and helium driver conditions of $p_4/p_o = 100$ and $T_4 = 300^0$ K.

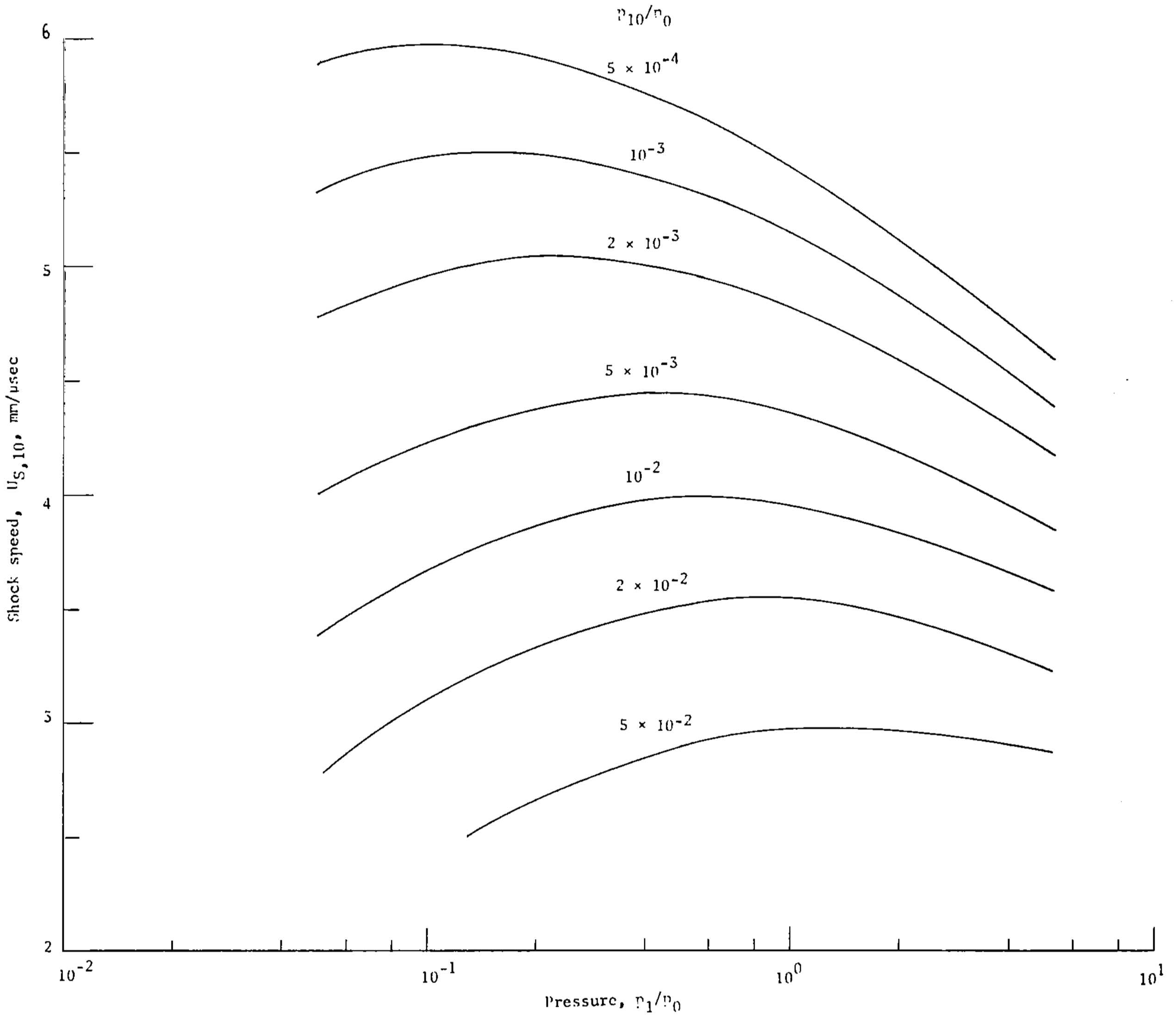

Figure 11.- Test gas shock speed as a function of buffer gas pressure for test gas of 90 percent N_2 and 10 percent CO_2 and hydrogen driver conditions of $p_4/p_0 = 100$ and $T_4 = 300^0$ K.